



XXV General Assembly and Congress of the International Union of Crystallography - IUCr 2021

August 14 - 22, 2021 | Prague, Czech Republic

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8:01:02pm CET

Radomír Kužel ▾

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Overview > Conference Agenda



Conference Agenda

Overview and details of the sessions of this conference. Please select a date or location to show only sessions at that day or location. Please select a single session for detailed view (with abstracts and downloads if available).

Please note that all times are shown in the time zone of the conference. **The current conference time is: 28th Dec 2024, 08:01:02pm CET**

Hide Presentations

Hide Downloads

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Table View

Authors

My Agenda

More...

Name, Title...

Filter by Area or Type of Session

All submission types / tracks

Session Overview

Date: Wednesday, 11/Aug/2021

School - Electron: Electron Crystallography School

Location: **virtual**

Session Chair: **Xiaodong Zou**

Session Chair: **Louisa Meshi**

Session Chair: **Lukáš Palatinus**

9:00am - 6:30pm

Website - virtual

Videos I: Introduction - Kolb: ADT - Hovmöller: RED

Videos II: Mugnaioli: From precession... - Abrahams: Continuous rotation... - Yonekura: 3D ED ...

Videos III: Hadermann: X-ray and electron... - Hovmöller: Symmetry... - Meshi: Unit cell ...

Videos IV: Xu: Sample preparation... - Nannenga: Data collection... - Willhammar: cRed data collection ...

Videos V: Gonen: MicroED... - Sponsors

The development of 3D ED on studying structure and charge state of protein microcrystals

Koji Yonekura

RIKEN / Tohoku University, Sayo, Japan

Unit cell and space group determination from ED and CBED

Louisa Meshi

Ben Gurion University of the Negev, Beer Sheva, Israel

External Resource:



Workshop - Data: When should small molecule crystallographers publish raw diffraction data?

Location: **virtual**

Session Chair: **Amy Sarjeant**

Session Chair: **Simon John Coles**

9:00am - 6:30pm

Website - virtual

Date: Thursday, 12/Aug/2021

School - Aperiodic: Workshop on Aperiodic and Magnetic Structure for Beginners

Location: **Institute of Physics, Czech Academy of Sciences**

Session Chair: **Márcel Petříček**

Session Chair: **Václav Henríques**

8:30am - 4:30pm

Website

Workshop CCDC/FIZ: CSD and ICSD workshop

Location: **virtual**

Session Chair: **Suzanna Ward**

Session Chair: **Annett Steudel**

9:00am - 4:00pm

Website

School - Electron 2: Electron Crystallography School

Location: **virtual**

Session Chair: **Xiaodong Zou**

Session Chair: **Louisa Meshi**

Session Chair: **Lukáš Palatinus**

9:00am - 6:30pm

Website

Videos I: Waterman: ED data processing... - Waterman: Dials...

Videos II: Diederichs: XDS software... - Smeets: Serial rotation...

Videos III: Sun: Phasing... - Palatinus: Kinematic and dynamic... - Puschmann: Olex2...

Videos IV: Uson: Phasing...macromolecules - McCoy: Phase... - Keegan: CCP4...

ED Data Processing theory

David Geoffrey Waterman

STFC, Didcot, United Kingdom

Different methods for phasing diffraction data – macromolecules

Isabel Usón¹, Claudia Millán³, Rafael J. Borges³, Logan S. Richards⁴, Maria D. Flores⁴, Michael R. Sawaya⁵, José A. Rodríguez⁴, George M. Sheldrick²

¹ICREA at IBMB-CSIC, Barcelona, Spain; ²University Göttingen, Germany; ³IBMB-CSIC; ⁴Department of Chemistry and Biochemistry; UCLA-DOE Institute for Genomics and Proteomics;(UCLA); Los Angeles, CA 90095, USA.; ⁵UCLA-DOE Institute for Genomics and Proteomics, Los Angeles, CA 90095, USA.

SEC - Posters: Electron Crystallography School - Poster



Location: **virtual**

Session Chair: **Xiaodong Zou**

Session Chair: **Louisa Meshi**

Session Chair: **Lukáš Palatinus**

Website

9:00am - 6:30pm

Quantitative analysis of diffuse electron scattering in the lithium-ion battery cathode material

$\text{Li}_{1.2}\text{Ni}_{0.13}\text{Mn}_{0.54}\text{Co}_{0.13}\text{O}_2$

Romy Poppe¹, Daphne Vandemeulebroucke¹, Reinhard B. Neder², Joke Hadermann¹

¹University of Antwerp, Department of Physics, Electron Microscopy for Materials Science (EMAT), Groenenborgerlaan 171, B-2020 Antwerp, Belgium; ²Friedrich-Alexander-Universität Erlangen-Nürnberg, Department of Physics, Institute of Condensed Matter Physics, Schloßplatz 4, 91054 Erlangen, Germany



[SEC - Posters-364-001_b.pdf](#)

Theoretical electrostatic potential maps of macromolecules calculated with multipolar electron scattering factors

Marta Kulik, Michał Leszek Chodkiewicz, Paulina Maria Dominiak

Biological and Chemical Research Centre, Department of Chemistry, University of Warsaw, Warsaw, Poland



[SEC - Posters-639-002_b.pdf](#)

Spinel ferrite nanoparticles in core shell architecture for heat release

Marco Sanna Angotzi

University of Cagliari, Cagliari, Italy



[SEC - Posters-644-003_b.pdf](#)

Refinements on electron diffraction data of β -glycine in MoPro: A quest for improved structure model

Kunal Kumar Jha¹, Barbara Gruza¹, Michał Leszek Chodkiewicz¹, Christian Jelsch², Paulina Maria Dominiak¹

¹University of Warsaw, Warsaw, Poland; ²Université de Lorraine, CNRS, CRM2, Nancy, France



[SEC - Posters-671-004_b.pdf](#)

Crystal structure of Zeolite A solved by Precession Electron Diffraction Tomography

Juan Ignacio Tirado Castaño¹, Jose Luis Jorda¹, Partha Pratim Das²

¹ITQ-UPV, Valencia, Spain; ²NanoMEGAS SPRL, Rue Émile Claus 49 bte 9, 1050, Brussels, Belgium



[SEC - Posters-988-005_b.pdf](#)

Investigating structure transformations of $\text{La}_x\text{Sr}_{2-x}\text{MnO}_{4.5}$ using *in situ* 3D electron diffraction in a gas environment

Daphne Vandemeulebroucke, Maria Batuk, Joke Hadermann

1EMAT, University of Antwerp, Groenenborgerlaan 171, B-2020 Antwerp, Belgium



[SEC - Posters-1399-006_b.pdf](#)

Scipion-ed: a workflow-based and self-documenting program for 3DED data processing

Viktor E. G. Bengtsson¹, José Miguel de la Rosa-Trevin², Laura Pacoste¹, Gerhard Hofer¹, Hongyi Xu¹, Xiaodong Zou¹

¹Department of Materials and Environmental Chemistry, Stockholm University, Stockholm; ²Department of Biochemistry and Biophysics, Science for Life Laboratory, Stockholm University, Stockholm



[SEC - Posters-1586-007_b.pdf](#)

Model dependence (IAM vs. TAAM) of B-factors - cases of X-ray and electron diffraction

Barbara Gruza¹, Christian Jelsch², Paulina Dominiak¹

¹University of Warsaw, Warszawa, Poland; ²CNRS: Vandoeuvre les Nancy, France



[SEC - Posters-1628-008_b.pdf](#)

On the Quality of Three-Dimensional Electron Diffraction Data for Direct Location of Guest Molecules in Open-Framework Materials

Meng Ge, Zhehao Huang, Hongyi Xu, Xiaodong Zou

Department of Materials and Environmental Chemistry, Stockholm University, 10691 Stockholm, Sweden; gemeng733@gmail.com



SEC - Posters-1650-009_b.pdf

Utilizing Scipion-ED for 3DED data processing

Laura C. Pacoste¹, Viktor E.G. Bengtsson¹, José Miguel de la Rosa-Trevín², Gerhard Hofer¹, Hongyi Xu¹, Xiaodong Zou¹

¹Stockholm University, Stockholm, Sweden; ²Department of Biochemistry and Biophysics, Science for Life Laboratory, Stockholm University; laura.pacoste@mmk.su.se



SEC - Posters-1592-010_b.pdf

Structural basis of higher-order assembly formation in Toll-like receptor 1,2 and 6 signaling pathway

YAN LI

The University of Queensland, St Lucia, Australia



SEC - Posters-1723-011_b.pdf

Prospects for improved quantitative electron diffraction.

Richard Beanland

University of Warwick, Coventry, United Kingdom



SEC - Posters-1678-012_b.pdf

Analysis of electrostatic interaction energies in complexes of IFIT5 proteins with RNA via UBDB+EPMM method

Urszula Anna Budniak, Paulina Maria Dominiak

Department of Chemistry, University of Warsaw, Warsaw, Poland; urszula.budniak@uw.edu.pl



SEC - Posters-1863-013_b.pdf

Polymorphism within molecular systems revealed by 3D electron diffraction.

Edward Thomas Broadhurst

The University of Edinburgh, Edinburgh, United Kingdom; s1371070@ed.ac.uk



SEC - Posters-1862-014_b.pdf

Unraveling unforeseen disorders in silicates with 3D electron diffraction

Jungyoun Cho, Xiaodong Zou, Tom Willhammar

Stockholm University, Stockholm, Sweden; jungyoun.cho@mmk.su.se

External Resource:



SEC - Posters-1647-015_b.pdf

Workshop - Data2: When should small molecule crystallographers publish raw diffraction data? (+)

Location: **virtual**

Session Chair: **Amy Sarjeant**

Session Chair: **Simon John Coles**

Website

9:00am - 6:30pm

Date: Friday, 13/Aug/2021

School - Aperiodic 2: Workshop on Aperiodic and Magnetic Structure for Beginners (+)

Location: **Institute of Physics, Czech Academy of Sciences**

Session Chair: **Václav Petříček**

Session Chair: **Margarida Henriques**

Website

8:30am - 4:30pm

Workshop - Olex: Olex2 workshop (+)

Location: **virtual**

Session Chair: **Horst Puschmann**

Website

8:30am - 4:30pm

School - Electron 3: Electron Crystallography School (+)

Location: **virtual**

Session Chair: **Xiaodong Zou**

9:00am - 5:00pm

Session Chair: **Louisa Meshi**
Session Chair: **Lukáš Palatinus**
Website

Videos I: Murshudov: Refinement of macromolecular... - Yamashita: Coot...
Videos III: Palatinus: PETS and Jana 2006... - Palatinus: Dynamic refinement...
Videos IV: Afonine: Phenix... - Afonine: Phenix-sof demo... QA.

Workshop - ICDD: ICDD workshop

9:00am - 5:00pm

Location: **virtual**
Session Chair: **Thomas Nelson Blanton**
Session Chair: **Jose Miguel Delgado**
Virtual workshop

Workshop - MSB: Methods of Structural Biology

12:30pm - 5:00pm

Location: **Biocev**
Session Chair: **Jan Dohnalek**
Session Chair: **Jan Stránský**
Website

Date: Saturday, 14/Aug/2021

Workshop - APEX: APEX4 Workshop (Bruker)

9:00am - 1:00pm

Location: **virtual**
Website - virtual

Workshop - MX: MX Raw image data and metadata, formats and validation

9:00am - 3:00pm

Location: **virtual**
Website

Workshop - WDQA: Data quality assesment

9:00am - 4:30pm

Location: **221-2**
Session Chair: **Julian Henn**
Website

School - Electron 4: Electron Crystallography School

2:00pm - 5:00pm

Location: **Club H**
Session Chair: **Xiaodong Zou**
Session Chair: **Louisa Meshi**
Session Chair: **Lukáš Palatinus**
Website

Video: Genderen: Detectors... - Bucker: Serial and scanning diffraction... - Beanland: Quantitative ED... - Dominiak: Potential in 3D ED... - Zou: 3D ED-MicroED...
Round table - Poster prizes -

Opening: Opening ceremony

5:30pm - 6:30pm

Session Chair: **Ivana Kuta Smatanova**
Session Chair: **Pavlaína Řezáčová**
Videos: Opening - IUCr president - CSCA - International Science Council

Opening music: Music

6:30pm - 7:00pm

Ensemble Website
Folk music - video

Ewald: Ewald prize lecture

7:00pm - 7:50pm

Session Chair: **Suzanna Ward**
Olga Kennard
Video

Celebrating Dr Olga Kennard

Suzanna Ward
The Cambridge Crystallographic Data Centre (CCDC), Cambridge, United Kingdom; ward@ccdc.cam.ac.uk

External Resource:



Ewald-1926-001_a.pdf

8:00pm - 10:00pm

Welcome: Welcome drink and refreshment

Location: **Exhibition and poster area**

Date: Sunday, 15/Aug/2021

KN-1: Quantum Crystallography: Past, Present, and Future

9:00am - 9:50am

Location: **Terrace 2A**
Session Chair: **Krzysztof Wozniak**
Dylan Jayatilaka

Quantum crystallography: past, present, and future

Dylan Jayatilaka
School of Molecular Sciences, The University of Western Australia 35 Stirling Highway, Crawley 6009, Perth, Western Australia ;
dylan.jayatilaka@uwa.edu.au

External Resource:



KN-1-1558-001_a.doc



KN-1-1558-001_b.pdf

9:00am - 9:50am

KN-2: The symbiosis of cryo-EM and X-ray crystallography in structure determination of large macromolecular systems

Location: **Terrace 2B**

Session Chair: **Marcin Nowotny**

Holger Stark

Atomic resolution structure determination by cryo-EM – where are the limits?

Holger Stark

Max-Planck-Institute for biophysical chemistry, Goettingen, Germany; hstark1@gwdg.de

External Resource:



KN-2-1643-001_b.pdf

9:00am - 9:50am

KN-3: High Pressure Crystallography Unlimited

Location: **Club A**

Session Chair: **Arthur Haozhe Liu**

Leonid Dubrovinsky

High pressure crystallography unlimited

Leonid Dubrovinsky

Bayreuth University, Bayreuth, Germany; leonid.dubrovinsky@uni-bayreuth.de

External Resource:



KN-3-1580-001_b.pdf

9:50am - 10:20am

Morning break 1: Exhibition, posters, coffee/tea

Location: **Exhibition and poster area**

MS-1: Structural bioinformatics

Location: **Club B**

Session Chair: **Janusz Marek Bujnicki**

Session Chair: **Jiri Cerny**

Invited: **Zhichao Miao (UK)**

Introduction

10:20am - 10:25am

Introduction to session

Janusz Bujnicki, Jiri Cerný 



MS-1-1728-001.pdf

10:20am - 12:45pm

10:25am - 10:55am

RNA-Puzzles - the evaluation and automation of RNA 3D structure prediction

Zhichao Miao^{1,2,3}

¹Translational Research Institute of Brain and Brain-Like Intelligence and Department of Anesthesiology, Shanghai Fourth People's Hospital Affiliated to Tongji University School of Medicine, Shanghai 200081, China; ²Newcastle Fibrosis Research Group, Institute of Cellular Medicine, Faculty of Medical Sciences, Newcastle University, Newcastle upon Tyne, UK; ³European Molecular Biology Laboratory, European Bioinformatics Institute (EMBL-EBI), Wellcome Genome Campus, Cambridge CB10 1SD, UK; zmiao@ebi.ac.uk

External Resource:



MS-1-580-002_b.pdf

10:55am - 11:25am

A nucleic acid structural alphabet and conformational analyses at dnatco.datmos.org

Bohdan Schneider

Institute of Biotechnology of the Czech Academy of Sciences, Vestec, Czech Republic

External Resource:



MS-1-713-003_b.pdf

11:25am - 11:45am

Applications of residue contact predictions in structural biology.

Filomeno Sanchez Rodriguez^{1,2}, **Ronan Keegan**³, **Melanie Vollmar**², **Gwynndaf Evans**², **Daniel Rigden**¹

¹University of Liverpool, Liverpool, United Kingdom; ²Life Science, Diamond Light Source, Harwell Science and Innovation Campus, Didcot, Oxfordshire, United Kingdom; ³STFC, Rutherford Appleton Laboratory, Harwell Oxford, United Kingdom; filomeno.sanchez-rodriguez@liverpool.ac.uk

External Resource:





MS-1-208-004_b.pdf

11:45am - 12:05pm

Pepsi-SAXS/SANS - small-angle scattering-guided tools for integrative structural bioinformatics

Sergei Grudinin¹, Anne Martel², Sylvain Prevost²

¹CNRS, Grenoble, France; ²ILL, Grenoble, France

External Resource:



MS-1-1285-005_b.pdf

12:05pm - 12:25pm

Refactoring the B-factor: intuitively extracting structural dynamics from macromolecular disorder

Nicholas M Pearce¹, Piet Gros²

¹Free University of Amsterdam, Amsterdam, The Netherlands; ²Utrecht University, Utrecht, The Netherlands

External Resource:



MS-1-700-006_b.pdf

12:25pm - 12:45pm

Computational modeling of RNA 3D structures and RNA-protein complexes, with the use of experimental data

Janusz Marek Bujnicki

International Institute of Molecular and Cell Biology in Warsaw, Warsaw, Poland; janusz@iimcb.gov.pl

External Resource:



MS-1-668-007_b.pdf

MS-2: Validation of cryoEM structures and maps

Location: **Club A**

Session Chair: **Jose-Maria Carazo**

Session Chair: **Elena Orlova**

Invited: **Florence Tama (Japan)**, **Pavel Afonine (USA)**, **G. Kleywegt (Germany)**

Session Abstracts

10:20am - 10:50am

Protein hydrogen bond parameters as a new validation tool

Pavel Afonine¹, Oleg Sobolev¹, Nigel Moriarty¹, Yanting Xu^{1,2}, Thomas Terwilliger^{3,4}, Paul Adams^{1,5}

¹Lawrence Berkeley National Laboratory, Berkeley, United States of America; ²International Center for Quantum and Molecular Structures, Shanghai University, Shanghai 200444, People's Republic of China; ³Bioscience Division, Los Alamos National Laboratory, Mail Stop M888, Los Alamos, NM 87545, USA; ⁴New Mexico Consortium, Los Alamos, NM 87544, USA; ⁵Department of Bioengineering, University of California Berkeley, Berkeley, CA 94720, USA; pafonine@lbl.gov

External Resource:



MS-2-126-001_b.pdf

10:50am - 11:20am

Integrative modeling to characterize structure and dynamics of biomolecules

Florence Tama

Nagoya University & RIKEN, Nagoya, Japan

External Resource:



MS-2-1234-002_b.pdf

11:20am - 11:50am

Community recommendations on validating cryo-EM models and data

Gerard Kleywegt

EMBL EBI, Cambridge, United Kingdom; gerard@ebi.ac.uk

External Resource:



10:20am - 12:45pm



MS-2-385-003_b.pdf

11:50am - 12:05pm

Cryo-EM Validation Metrics in EMDA

Rangana Warshamanage, Keitaro Yamashita, Garib N. Murshudov

MRC Laboratory of Molecular Biology, Francis Crick Avenue, Cambridge, Biomedical Campus, Cambridge, CB2 0QH, UK

External Resource:



MS-2-1256-004_b.pdf

12:05pm - 12:20pm

FSC-Q: A method for quality analysis of cryoEM-derived models

Erney Ramirez-Aportela, David Maluenda, Yuniur C. Fonseca, Pablo Conesa, Roberto Marabini, Carlos Oscar S. Sorzano, Jose M. Carazo

CNB-CSIC, Madrid, Spain; erney.ramirez@gmail.com

External Resource:



MS-2-1095-005_b.pdf

12:20pm - 12:35pm

Outcomes from EMDDataResource model challenges

Catherine Lawson¹, Andriy Kryshstafovych², Wah Chiu³

¹Rutgers University, NJ, USA; ²University of California Davis, CA, USA; ³Stanford University/SLAC, Stanford, CA, USA

External Resource:



MS-2-1294-006_b.pdf

12:35pm - 12:50pm

Quantifying resolvability of atomic features in cryo-EM maps using Q-scores

Greg Pintilie¹, Michael Schmid², Wah Chiu³

¹Stanford University; ²Stanford University, SLAC National Accelerator Laboratory; ³Stanford University, SLAC National Accelerator Laboratory; gregdp@stanford.edu

External Resource:



MS-2-1174-007_b.pdf

MS-3: Crystallographic approaches for designing new framework materials (including post-synthetic modification)

Location: **223-4**

Session Chair: **Yue-Biao Zhang**

Session Chair: **Sergei Alexandrovich Sapchenko**

10:20am - 10:25am

Introduction to session

Yue-Biao Zhang, Sergei Alexandrovich Sapchenko



MS-3-1733-001.pdf

10:25am - 10:55am

From positive to colossal negative thermal expansion in a novel family of bimetallic imidazoles

Sanja Burazer¹, Lukáš Horák¹, Yaroslav Filinchuk³, Milan Dopita¹, Radovan Černý², Jasminka Popović⁴

¹MFF, Charles University, Prague, Czech Republic; ²DQMP, University of Geneva, Geneva, Switzerland; ³ICMN, Université catholique de Louvain, Louvain-la-Neuve, Belgium; ⁴Ruder Bošković Institute, Zagreb, Croatia; Sanja.Burazer@irb.hr



MS-3-1039-002_b.pdf

10:55am - 11:25am

Solvent-dependent phases and phase transformations of a family of 2D halogen-bonded networks

Thomas Michael Roseveare, Conor Wilde, Vivien Csonka, Lee Brammer

The University of Sheffield, Sheffield, United Kingdom; tom.roseveare@sheffield.ac.uk

External Resource:



10:20am - 12:45pm



MS-3-394-003_b.pdf

11:25am - 11:45am

Structural features of the formation of Hydrogen bonded Organic Frameworks

Petra Bombicz¹, Laura Bereczki², Nóra V. May¹, Roberta Palkó³, Tamás Holczbauer⁴

¹Centre for Structural Science, Research Centre for Natural Sciences; ²Centre for Structural Science and Institute of Materials and Environmental Chemistry, Research Centre for Natural Sciences; ³Institute of Organic Chemistry, Research Centre for Natural Sciences; ⁴Centre for Structural Science and Institute of Organic Chemistry, Research Centre for Natural Sciences, Budapest, Hungary; bombicz.petra@tk.mta.hu

External Resource:



MS-3-1237-004_b.pdf

11:45am - 12:05pm

Preferences of Chirality and Polarity in Triglycine sulfate Crystals

Yukana Terasawa¹, Toshio Kikuta², Masaaki Ichiki³, Sota Sato⁴, Kazuhiko Ishikawa⁵, Toru Asahi^{6,7}

¹School of Advance Science and Engineering, Waseda University, Tokyo, Japan; ²Faculty of Engineering, University of Toyama, Toyama, Japan; ³Research Center for Ubiquitous MEMS and Micro Engineering, National Institute of Advanced Industrial Science and Technology (AIST), Ibaraki, Japan; ⁴Department of Applied Chemistry, School of Engineering, The University of Tokyo, Tokyo, Japan; ⁵Graduate School of Advance Science and Engineering, Waseda University, Tokyo, Japan; ⁶Faculty of Science and Engineering, Waseda University, Tokyo, Japan; ⁷Research Organization for Nano & Life Innovation, Waseda University, Tokyo, Japan; tinkerbell@akane.waseda.jp



MS-3-529-005_b.pdf

12:05pm - 12:25pm

Solid-state isolation of reactive complexes in a metal-organic framework matrix

Ricardo PERALTA, Michael HUXLEY, Jorge ALBALAD, Christian DOONAN, **Christopher SUMBY**

Department of Chemistry, The University of Adelaide, Adelaide, Australia; christopher.sumby@adelaide.edu.au



MS-3-740-006_b.pdf

12:25pm - 12:45pm

Improvement of precision and sensitivity in refinement of crystal structure factors using zone-axis and Bragg-excited CBED patterns

Bikas Aryal¹, Daisuke Morikawa¹, Kenji Tsuda², Masami Terauchi¹

¹IMRAM, Tohoku University, Sendai, Japan.; ²FRIS, Tohoku University, Sendai, Japan.; aryla.bikas.p4@dc.tohoku.ac.jp



MS-3-593-007_b.pdf

MS-4: Quantum crystallography challenges and newest accomplishments

Location: **Club C**

Session Chair: **PIERO MACCHI**

Session Chair: **Dietmar Stalke**

Invited: **Alessandro Genoni** (France), **Nicolas Claiser** (France)

Introduction

10:20am - 10:25am

Introduction to session

Piero Macchi, **Dietmar Stalke**



MS-4-1734-001.pdf

10:25am - 10:55am

Multi-determinant X-ray restrained wavefunction approaches

Alessandro Genoni

CNRS & University of Lorraine, Metz, France; Alessandro.Genoni@univ-lorraine.fr

External Resource:



MS-4-778-002_b.pdf

10:55am - 11:25am

Spin resolved charge density and wave function refinements: the Mollynx/MoPro software

Mohamed SOUHASSOU¹, Iurii KIBALIN², Ariste Bolivard VOUPACK³, Peter BLAHA⁴, Claude LECOMTE¹, **Nicolas CLAISER**¹

10:20am - 12:45pm

¹Université de Lorraine and CNRS, CRM2, BP 70239, 54506 Vandœuvre-lès-Nancy, France; ²Laboratoire Léon Brillouin, CEA-CNRS, CE-Saclay, 91191 Gif-sur-Yvette, France; ³URMACETS, Département de Physique, Université de Dschang, BP 67 Dschang, Cameroun.; ⁴Institut für Materialchemie, TU Wien, Getreidemarkt 91060 Wien, Austria; nicolas.claiser@univ-lorraine.fr

External Resource:



MS-4-921-003_b.pdf

11:25am - 11:45am

N-representable one-electron reduced density Matrices reconstruction at non-zero temperatures.

Yoann Levis Launay¹, Jean-Michel Gillet²

¹CentraleSupélec (Paris-Saclay University), Gif-sur-Yvette, France; ²Structures, Properties and Modeling of Solids, CentraleSupélec (Paris-Saclay University), Gif-sur-Yvette, France; yoann.launay@student-cs.fr

External Resource:



MS-4-473-004_b.pdf

11:45am - 12:05pm

Accurate refinement of hydrogen atoms positions through a quantum mechanical embedding scheme based on extremely localized molecular orbitals

Giovanni Macetti, Erna Katharina Wieduwilt, Alessandro Genoni

University of Lorraine & CNRS, Metz, France; giovanni.macetti@univ-lorraine.fr

External Resource:



MS-4-793-005_b.pdf

12:05pm - 12:25pm

Relativistic Hirshfeld atom refinement of organo-gold(I) and organo-mercury(II) compounds.

Sylwia Pawłędzio¹, Maura Malinska¹, Florian Kleemiss², Simon Grabowsky², Krzysztof Woźniak¹

¹Biological and Chemical Research Centre, Department of Chemistry, University of Warsaw, Poland.; ²University of Bern, Department of Chemistry and Biochemistry, Freiestrasse 3, 3012 Bern, Switzerland.; spawledzio@uw.edu.pl

External Resource:



MS-4-443-006_b.pdf

MS-5a: Crystal structure prediction

Location: **Terrace 2A**

Session Chair: **Qiang Zhu**

Invited: Ivan Kruglov (Russia), Graeme Day (UK)

Introduction

10:20am - 10:25am

Introduction to session

Qiang Zhu, **Rajeev Ahuja**



MS-5a-1735-001.pdf

10:25am - 10:55am

T-USPEX - novel method for crystal structure prediction at finite temperatures

Ivan Kruglov^{1,2}, Alexey Yanilkin^{1,2}, Artem Oganov^{3,1,2,4}

¹Dukhov Research Institute of Automatics (VNIIA), Moscow, Russia; ²Moscow Institute of Physics and Technology, Dolgoprudny, Russia; ³Skolkovo Institute of Science and Technology, Moscow, Russia; ⁴Northwestern Polytechnical University, Xi'an, China; ivan.kruglov@phystech.edu

External Resource:



MS-5a-577-002_b.pdf

10:55am - 11:25am

Functional materials exploration through evolutionary searching and large-scale crystal structure prediction

Graeme M Day, Josh E. Campbell, Chi Y. Cheng

University of Southampton, Southampton, United Kingdom; g.m.day@soton.ac.uk

External Resource:



10:20am - 12:45pm



MS-5a-969-003_b.pdf

11:25am - 11:45am

Design of metal-organic frameworks: from theoretical structure and reactivity predictions to mechanochemical synthesis and screening

Yizhi Xu¹, James Darby², Joseph Marrett³, Hatem Titi³, Tomislav Friščić³, Andrew Morris⁴, Mihails Arhangel'skis¹

¹Faculty of Chemistry, University of Warsaw, Warsaw 02-093, Poland; ²Engineering Department, University of Cambridge, Cambridge CB2 1PZ, U.K.; ³Department of Chemistry, McGill University, Montreal H3A 0B8, Canada; ⁴School of Metallurgy and Materials, University of Birmingham, Edgbaston, Birmingham B15 2TT, U.K.; y.xu7@student.uw.edu.pl

External Resource: Presentation



MS-5a-902-004_b.pdf

11:45am - 12:05pm

CCDCGAN: Deep learning prediction of crystal structures

Hongbin Zhang, Teng Long, Yixuan Zhang, Nuno Fortunato, Chen Shen, Oliver Gutfleisch

Institute of Materials Science, Technical University of Darmstadt, 64287 Darmstadt, Germany; hongbin.zhang@tu-darmstadt.de

External Resource: Presentation



MS-5a-904-005_b.pdf

12:05pm - 12:25pm

Computational design and prediction of solid-state properties of metal-organic frameworks

Mihails Arhangel'skis¹, Yizhi Xu¹, James P. Darby², Novendra Novendra³, Joseph M. Marrett⁴, Athanassios D. Katsenis⁴, Hatem M. Titi⁴, Andrew J. Morris⁵, Tomislav Friščić⁴, Alexandra Navrotsky^{3,6}

¹University of Warsaw, Warsaw, Poland; ²Department of Engineering, University of Cambridge; ³Peter A. Rock Thermochemistry Laboratory and NEAT ORU, University of California Davis; ⁴Department of chemistry, McGill University; ⁵School of Metallurgy and Materials, University of Birmingham; ⁶School of Molecular Sciences and Center for Materials of the Universe, Arizona State University; m.arhangel'skis@uw.edu.pl

External Resource: Presentation



MS-5a-873-006_b.pdf

12:25pm - 12:45pm

Computational search for new high- T_C superconductors based on lanthanoid and actinoid hydrides at moderate pressures

Alexander Kvashnin¹, Dmitrii Semenok¹, Ivan Kruglov^{2,3}, Artem Oganov^{1,2,3,4}

¹Skolkovo Institute of Science and Technology, Moscow, Russian Federation; ²Dukhov Research Institute of Automatics (VNIIA); ³Moscow Institute of Physics and Technology; ⁴Northwestern Polytechnical University; A.Kvashnin@skoltech.ru

External Resource: Presentation



MS-5a-176-007_b.pdf

MS-6: Application of electron crystallography to functional materials

Location: **Terrace 2B**

Session Chair: **Holger Klein**

Session Chair: **Karla Balzuweit**

Invited: **Mauro Gemmi (Italy)**, **Maria Roslova (Germany)**

Introduction

10:20am - 10:25am

Introduction to session

Holger Klein, **Karla Balzuweit**



MS-6-1736-001.pdf

10:25am - 10:55am

3D electron diffraction on nanoparticles with a complex structure.

Mauro Gemmi¹, Enrico Mugnaioli¹, Roman Kaiukov², Stefano Toso², Luca De Trizio², Liberato Manna²

¹Center for Nanotechnology Innovation@NEST, Istituto Italiano di Tecnologia, Pisa, Italy; ²Department of Nanochemistry, Istituto Italiano di Tecnologia, Genova, Italy; mauro.gemmi@iit.it

External Resource: Presentation

10:20am - 12:45pm



MS-6-939-002_b.pdf

10:55am - 11:25am

Reliable structure determination of K-intercalated RuCl_3 nanoflakes by 3D electron crystallography and multivariate analysis of fused EELS and EDX spectrum images

M. Roslova^{1,3}, T. Thersleff¹, E. Vinokurova², S. Avdoshenko³, A. Isaeva^{3,4}

¹Department of Materials and Environmental Chemistry, Stockholm University, Stockholm, Sweden; ²Department of Physics, Technische Universität Dresden, Germany; ³Institute for Solid State and Materials Research (IFW) Dresden, Germany; ⁴Institute of Physics, University of Amsterdam, The Netherlands; m.roslova@ifw-dresden.de

External Resource:



MS-6-1135-003_b.pdf

11:25am - 11:50am

3D- Δ PDF from electron diffraction data

Ella Mara Schmidt¹, Yasar Krysiak^{2,3}, Paul Benjamin Klar², Lukas Palatinus², Reinhard B. Neder⁴, Andrew L. Goodwin¹

¹Inorganic Chemistry, University of Oxford, United Kingdom; ²Department of Structural Analysis, Institute of Physics of the CAS, Prague, Czechia; ³Institute of Inorganic Chemistry of the Leibniz University Hannover, Germany; ⁴Kristallographie und Strukturphysik, Friedrich-Alexander-Universität, Erlangen, Germany; ella.schmidt@chem.ox.ac.uk

External Resource:



MS-6-816-004_b.pdf

11:50am - 12:15pm

Electron diffraction for the promotion of stable and green metal-organic frameworks

Erik Svensson Grape¹, Tania Hidalgo², Patricia Horcajada², Ilich A. Ibarra³, A. Ken Inge¹

¹Stockholm University, Stockholm, Sweden; ²IMDEA Energy, Madrid, Spain; ³Universidad Nacional Autónoma de México, Mexico City, Mexico; andrew.inge@mmk.su.se

External Resource:



MS-6-1058-005_b.pdf

12:15pm - 12:40pm

Crystal structure of the $\text{Al}_{78}\text{Mn}_{17.5}\text{Pt}_{4.5}$ phase as revealed by electron crystallography

Louisa Meshi¹, Rimón Tamari¹, Benjamin Grushko^{2,3}

¹Ben Gurion University of the Negev, Beer Sheva, Israel; ²MaTeCK GmbH, 52428 Jülich, Germany; ³Peter-Grünberg-Institut, Forschungszentrum Jülich, 52425 Jülich, Germany; louisa@bgu.ac.il

External Resource:



MS-6-1335-006_b.pdf

MS-7: High throughput vs. careful planning: How to get the best data?

Location: **Club H**

Session Chair: **John Richard Helliwell**

Session Chair: **Selina Lea Sophie Storm**

Invited: **Danny Axford (UK)**, **Aina Cohen (USA)**

Introduction

10:20am - 10:25am

Introduction to session

John Richard Helliwell, Selina Lea Sophie Storm



MS-7-1737-001.pdf

10:25am - 10:55am

Next-generation Automation and Remote-access Crystallography

Aina Cohen

Stanford Synchrotron Radiation Lightsource (SSRL) and Linac Coherent Light Source (LCLS), SLAC National Accelerator Laboratory, Stanford University, Menlo Park, United States of America; ACohen@SLAC.Stanford.edu

External Resource:



10:20am - 12:45pm



MS-7-1359-002_b.pdf

10:55am - 11:25am

Strength in Numbers: Exploiting the space between single crystal oscillation and serial femtosecond crystallography

Danny Axford, Sam Horrell, Robin Leslie Owen

Diamond Light Source, Harwell Oxford, Didcot, OX11 0DE, United Kingdom; danny.axford@diamond.ac.uk

External Resource:



MS-7-1011-003_b.pdf

11:25am - 11:45am

Towards High-Throughput Autonomous Infrared Spectromicroscopy

Petrus Zwart, Liang Chen, Marcus Noack, Steven Lee, Patricia Valdespino Castillo, Hoi-Ying Holman

LBNL, Berkeley, United States of America; phzwart@lbl.gov

External Resource:



MS-7-1001-004_b.pdf

11:45am - 12:05pm

Strategy in the age of 360° sweeps

Andreas Förster, Marcus Müller, Clemens Schulze-Bries

DECTRIS, Baden-Dättwil, Switzerland; andreas.foerster@dectris.com

External Resource:



MS-7-674-005.pdf

12:05pm - 12:25pm

Exploring the mechanism of elastically flexible crystals by automatic analysis

Amy Jayne Thompson^{1,2}, Jason Price², Kate Smith², Jack Clegg¹

¹The University of Queensland, St Lucia, QLD, Australia; ²The Australian Synchrotron, Clayton, VIC, Australia;

amy.thompson2@uqconnect.edu.au

External Resource:



MS-7-222-006_b.pdf

Finding the optimal resolution cutoff with PAIREF

Martin Malý^{1,2}, Kay Diederichs³, Jan Stránský², Kristýna Adámková^{2,4}, Tereza Skálová², Jan Dohnálek², Petr Kolenko^{1,2}

¹Czech Technical University in Prague, Czech Republic, Faculty of Nuclear Sciences and Physical Engineering; ²Institute of Biotechnology of the Czech Academy of Sciences, Biocev; ³University of Konstanz; ⁴University of Chemical and Technology Prague, Department of Biochemistry and Microbiology; martin.maly@jfi.cvut.cz

External Resource:



MS-7-686-007_b.pdf

MS-8: Social media and new frontiers for spreading crystallographic

Location: Club D

Session Chair: Andrea Ienco

Session Chair: Helen Maynard-Casely

Invited: Delphine Chenevier (France), Rhiannon Morris (Australia)

Introduction

10:20am - 10:25am

Introduction to session

Andrea Ienco, Helen Maynard-Casely



MS-8-1738-001.pdf

10:25am - 10:55am

Humanising science to reach new audience

Delphine CHENEVIER

10:20am - 12:45pm

ESRF, Grenoble, France; delphine.chenevier@esrf.fr

External Resource:



MS-8-684-002_b.pdf

10:55am - 11:25am

Using social media to make crystallography accessible

Rhiannon Morris

Walter and Eliza Hall Institute, Parkville, Australia; morris.r@wehi.edu.au

External Resource:



MS-8-198-003_b.pdf

11:25am - 11:45am

Using social media to share the wonders of crystallography - perspectives from a structural database

Ilaria Gimondi, Yinka Olatunji-Ojo, Zainab Abdulali, Ana Machado, Sophie Bryant, Suzanna Ward
Cambridge Crystallographic Data Centre, Cambridge, United Kingdom; igimondi@ccdc.cam.ac.uk

External Resource:



MS-8-1131-004_b.pdf

11:45am - 12:05pm

Memes: a new avenue for spreading crystallographic knowledge for the next generation

Sneh Patel^{1,2}, Martin Spasovski^{1,2}, Andrew Chan^{1,2}, Dana Goodacre^{1,2}, Timothy Christopher^{1,2}, Rosanna Rov^{1,2}, Mark Smith^{1,2}, Ryan Silk^{1,2}, Tilo Söhnel^{1,2}

¹School of Chemical Sciences, University of Auckland, 23 Symonds Street, Auckland 1010, New Zealand; ²Macdiarmid Institute for Advanced Materials and Nanotechnology, Victoria University of Wellington, Wellington 6140, New Zealand; spt796@aucklanduni.ac.nz

External Resource:



MS-8-384-005_b.pdf

12:05pm - 12:25pm

The Building Blocks of Battery Technology: Inspiring the next generation of battery researchers

Elizabeth Helen Driscoll¹, Ruth Patchett², Emily Hayward¹, Paul Anderson¹, Emma Kendrick³, Peter Raymond Slater¹

¹School of Chemistry, The University of Birmingham, Edgbaston, B15 2TT, UK; ²School of Education, The University of Birmingham, Edgbaston, B15 2TT, UK; ³School of Metallurgy and Materials, The University of Birmingham, Edgbaston, B15 2TT, UK; ehd345@student.bham.ac.uk

External Resource:



MS-8-1043-006_b.pdf

12:25pm - 12:45pm

Social media for the growth of a scientific community: the case of the Italian Young Crystallographers Group

Paolo Pio Mazzeo

University of Parma, Parma, Italy; paolopio.mazzeo@unipr.it

External Resource:



MS-8-1100-007_b.pdf

SMS-1: Session in the memory of An-Pang Tsai: from quasicrystals to catalysis

Location: 221-2

Session Chair: Marc de Boissieu

Session Chair: Yasushi Ishii

Introduction

10:20am - 10:25am

Introduction to session

Marc de Boissieu, **Yasushi Ishii**



SMS-1-1835-001.pdf

10:20am - 12:45pm

10:25am - 10:45am

An-Pang Tsai: an exceptional career from quasicrystals to catalysis

Marc de Boissieu

Univ. Grenoble Alpes, CNRS, Grenoble INP, SIMAP F-38000, Grenoble France; marc.de-boissieu@simap.grenoble-inp.fr

External Resource:



[SMS-1-1661-002_b.pdf](#)

10:45am - 11:15am

Structure of Tsai-type icosahedral quasicrystals

Hiroyuki Takakura

Division of Applied Physics, Faculty of Engineering, Hokkaido University, Sapporo, Japan; takakura@eng.hokudai.ac.jp

External Resource:



[SMS-1-1037-003_b.pdf](#)

11:15am - 11:45am

Heritage from Professor An Pang Tsai to the research field of metallic catalysis materials

Satoshi KAMEOKA

Tohoku University, Sendai, Japan; satoshi.kameoka.b4@tohoku.ac.jp

External Resource:



[SMS-1-1244-004_b.pdf](#)

11:45am - 12:05pm

An Pang Tsai – a chemist

Yuri Grin

Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany; grin@cpfs.mpg.de

External Resource:



[SMS-1-1667-005_b.pdf](#)

12:05pm - 12:25pm

Epitaxial Thin Films on Tsai-type Quasicrystals

Hem Raj Sharma, Sam Coates, Sanger Hars, Ronan McGrath

The University of Liverpool, Liverpool, United Kingdom; h.r.sharma@liv.ac.uk

External Resource:



[SMS-1-1200-006_b.pdf](#)

12:25pm - 12:45pm

An-Pang Tsai, a scientist, inspirator and friend

Sven Lidin¹, Julia Maria Hübner²

¹Lund University, Lund, Sweden; ²Lund University, Lund, Sweden; sven.lidin@chem.lu.se

External Resource:



12:45pm - 2:45pm	ECA-0: ECA EC meeting Session Chair: Udo Heinemann Session Chair: Arie van der Lee ECA EC meeting	⊕
12:45pm - 2:45pm	Lunch 1: Exhibition, posters, lunches Location: Exhibition and poster area	⊕
1:30pm - 2:30pm	CS-1: Commercial session: Bruker / Incoatec Location: Terrace 2A Session Chair: Martin Adam Session Chair: Joerg Wiesmann 60 min company presentation Videos: M. Adam - V. Smith - R. Durst - J. Graf	⊕
2:45pm - 3:45pm	MS-5b: Crystal structure prediction Location: 223-4 Session Chair: Qiang Zhu Session Chair: Rajeev Ahuja	⊕

2:45pm - 3:05pm

Le mieux est l'ennemi du bon; homology modelling with Phyre2 in a deep learning world

Harold R. Powell, Michael J.E. Sternberg, Lawrence A. Kelley
Imperial College London, United Kingdom; harry@hp-crystal.com

External Resource:



MS-5b-1270-001_b.pdf

3:05pm - 3:25pm

Prediction of the atomic structure of two-dimensional materials on substrates

Arslan B. Mazitov^{1,3}, Artem R. Oganov²

¹Moscow Institute of Physics and Technology, 9 Institutsky lane, Dolgoprudny 141701, Russian Federation; ²Skolkovo Institute of Science and Technology, Skolkovo Innovation Center, 3 Nobel Street, Moscow 121205, Russian Federation; ³Dukhov Research Institute of Automatics (VNIIA), Moscow 127055, Russian Federation; arslan.mazitov@phystech.edu

External Resource:



MS-5b-820-002_b.pdf

3:25pm - 3:45pm

Nucleating different coordination in crystal under pressure: Study of B1-B2 transition in NaCl by metadynamics

Matej Badin^{1,2}, Roman Martoňák²

¹SISSA – Scuola Internazionale Superiore di Studi Avanzati, Via Bonomea 265, 34136 Trieste, Italy; ²Department of Experimental Physics, Comenius University, Mlynská Dolina F2, 842 48 Bratislava, Slovakia; mbadin@sissa.it

External Resource:



MS-5b-1066-003_b.pdf

MS-09: Structure guided drug design and antibiotic resistance targets

Location: **Club A**

Session Chair: **Begoña Heras**

Session Chair: **Anton V. Zavialov**

Invited: **Vibha Gupta (India)**, **Jade Forwood (Australia)**

Introduction

2:45pm - 2:50pm

Introduction to session

Begoña Heras, Anton V. Zavialov



MS-09-1739-001.pdf

2:50pm - 3:20pm

Understanding viral host interactions that modulate nuclear transport and innate immunity

S. Tsimbalyuk¹, K.M. Smith¹, M.R. Edwards², J. Batra², T.P. Soares da Costa³, D. Aragao⁴, C.F. Basler², **J.K. Forwood¹**

¹School of Biomedical Sciences, Charles Sturt University, Wagga Wagga, NSW, Australia; ²Center for Microbial Pathogenesis, Institute for Biomedical Sciences, Georgia State University, Atlanta, USA; ³Department of Biochemistry and Genetics, La Trobe Institute for Molecular Science, La Trobe University, Melbourne, VIC, Australia; ⁴Australian Synchrotron, Australian Nuclear Science and Technology Organisation, 800 Blackburn Road, Clayton, VIC, Australia

External Resource:



MS-09-1396-002_b.pdf

3:20pm - 3:50pm

Novel targets in old rouges: Integrative structural biology approach for discovery of natural product inhibitors

Vibha Gupta, Monika Antil, Sunita Gupta, Deepali Verma, Juhi Mathur

Jaypee Institute of Information Technology, A-10, Sector-62, Noida, U.P., India; vibha.gupta@jiit.ac.in

External Resource:



MS-09-1563-003_b.pdf

3:50pm - 4:10pm

The structure of the ABC transporter PsABC shows that bacterial manganese import is achieved by unique architectural features that are conserved across the kingdoms of life.

2:45pm - 5:10pm

Stephanie L. Neville¹, Jennie Sjöhamn², Jacinta A. Watts¹, Hugo MacDermott-Opeskin³, Stephen J. Fairweather³, Katherine Ganio¹, Alex Carey Hulyer¹, Andrew J. Hayes¹, Aaron P. McGrath¹, Tess. R. Malcolm¹, Mark R. Davies¹, Norimichi Nomura⁴, Iwata So⁴, Megan L. O'Mara³, Christopher A. McDavitt¹, **Megan J. Maher**¹

¹The University of Melbourne, Parkville, Australia; ²University of Gothenburg, Gothenburg, Sweden.; ³Australian National University, Canberra, Australia; ⁴Kyoto University, Kyoto, Japan

External Resource:



MS-09-1026-004_b.pdf

4:10pm - 4:30pm

Uncovering the structures and mechanisms for the largest group of bacterial surface virulence factors.

Jason Paxman¹, Julieanne Vo¹, Gabriella Martínez Ortiz¹, Makrina Totsika², Alvin Lo³, Lilian Hor¹, Santosh Panjikar⁴, Mark Schembri³, Begoña Heras¹

¹Department of Biochemistry and Genetics, La Trobe Institute for Molecular Science, La Trobe University, Melbourne, Victoria, Australia; ²Institute of Health and Biomedical Innovation, School of Biomedical Sciences, Queensland University of Technology, Herston, Queensland, Australia; ³Australian Infectious Diseases Research Centre, School of Chemistry and Molecular Biosciences, The University of Queensland, Brisbane, Queensland, Australia; ⁴Macromolecular Crystallography, Australian Synchrotron, Clayton, Victoria, Australia; j.paxman@latrobe.edu.au

External Resource:



MS-09-1347-005_b.pdf

4:30pm - 4:50pm

Inhibiting, stabilising and probing the function of the Retromer endosomal trafficking complex through the novel macrocyclic peptides

Kai-En Chen¹, Qian Guo¹, Timothy A. Hill¹, Yi Cui², Amy K. Kendall³, Natalya Leneva⁴, Zhe Yang², David P. Fairlie¹, Hiroaki Suga⁵, Lauren P. Jackson³, Rohan D. Teasdale², Toby Passioura⁶, Brett M. Collins¹

¹The University of Queensland, Institute for Molecular Bioscience, St. Lucia, Queensland, 4072, Australia; ²The University of Queensland, School of Biomedical Sciences, St Lucia, Queensland, 4072, Australia; ³Department of Biological Sciences, Center for Structural Biology, Vanderbilt University, Nashville, TN 37232, USA; ⁴Cambridge Institute for Medical Research, University of Cambridge, Cambridge, UK; ⁵Department of Chemistry, Graduate School of Science, the University of Tokyo, 7-3-1 Hongo, Bunkyo-Ku, Tokyo 113-0033, Japan; ⁶Sydney Analytical, the University of Sydney, Camperdown, New South Wales 2050, Australia

External Resource:



MS-09-839-006_b.pdf

4:50pm - 5:10pm

Structural and mechanistic studies on carbapenem-hydrolysing class D serine β -lactamases leading to improved inhibitor design

Clyde Smith¹, Nichole Stewart², Marta Toth², Sergei Vakulenko²

¹Stanford Synchrotron Radiation Lightsource, Stanford University, Menlo Park, California, USA; ²Department of Chemistry and Biochemistry, University of Notre Dame, Notre Dame, Indiana, USA

External Resource:



MS-09-183-007_b.pdf

MS-10: Structural biology of eukaryotic immune systems

Location: **Club B**

Session Chair: **Bostjan Kobe**

Session Chair: **Savvas Savvides**

Invited: **Tsan Sam Xiao** (USA), Raul Olivier Martin (USA), Wen Song (Germany)

Introduction

2:45pm - 2:50pm

Introduction to session

Bostjan Kobe, **Savvas Savvides**



MS-10-1740-001.pdf

2:50pm - 3:20pm

Catching fire: inflammatory responses mediated by inflammasomes, caspases, and gasdermins

Zhonghua Liu¹, Chuanping Wang¹, Jie Yang², **Tsan Sam Xiao**¹

¹Case Western Reserve University, Cleveland, OH, USA; ²The Scripps Research Institute, La Jolla, CA, USA.

External Resource:





MS-10-1018-002_b.pdf

3:20pm - 3:50pm

Structure of the activated ROQ1 resistosome directly recognizing the pathogen effector XopQ

Raoul Olivier Martin^{1,3,4}, **Tiancong Qi**^{2,3,4}, **Haibo Zhang**², **Furong Liu**^{3,4}, **Miles King**^{3,4}, **Claire Toth**⁵, **Eva Nogales**^{5,6,7}, **Brian Staskawicz**^{3,4}

¹Biophysics Graduate Group, University of California, Berkeley, CA 94720, USA; ²Center for Plant Biology, School of Life Sciences, Tsinghua University, Beijing 100084, China.; ³Department of Plant and Microbial Biology, University of California, Berkeley, CA 94720 USA; ⁴Innovative Genomics Institute, University of California, Berkeley, CA 94720 USA.; ⁵Department of Molecular and Cellular Biology, University of California, Berkeley, CA 94720, USA; ⁶Howard Hughes Medical Institute, University of California, Berkeley, CA 94720, USA.; ⁷Molecular Biophysics and Integrated Bioimaging Division, Lawrence Berkeley National Laboratory, University of California, Berkeley, CA 94720, USA.

External Resource:



MS-10-1369-003_b.pdf

3:50pm - 4:20pm

Structural mechanism of NAD⁺ cleavage by plant TIR domain

Wen Song

Max Planck Institute for Plant Breeding Research, Köln, Germany

External Resource:



MS-10-1367-004_b.pdf

4:20pm - 4:40pm

The structure of the marsupial $\gamma\mu$ T cell receptor defines a third T cell lineage in vertebrates

Kim Morrissey¹, **Marcin Wegrecki**², **Praveena Thirunavukkarasu**^{2,3}, **Victoria Hansen**¹, **Komagal Sivaraman**², **Sam Darko**⁴, **Daniel Douek**⁴, **Jamie Rossjohn**^{2,3,5}, **Robert Miller**¹, **Jerome Le Nours**^{2,3}

¹Center for Evolutionary & Theoretical Immunology, Department of Biology, University of New Mexico, Albuquerque, NM, USA; ²Infection and Immunity Program and Department of Biochemistry and Molecular Biology, Biomedicine Discovery Institute, Monash University, Clayton, Victoria, Australia; ³Australian Research Council Centre of Excellence in Advanced Molecular Imaging, Monash University, Clayton, Victoria, 3800, Australia; ⁴Human Immunology Section, Vaccine Research Center, National Institute of Allergy and Infectious Diseases, National Institutes of Health, Bethesda, MD, USA; ⁵Institute of Infection and Immunity, Cardiff University School of Medicine, Heath Park, Cardiff, CF14 4XN, UK

External Resource:



MS-10-1036-005_b.pdf

4:40pm - 5:00pm

Bacterial lipopolysaccharide recognition by surfactant protein D

Annette K Shrive¹, **Jamie R Littlejohn**^{1,2}, **Harry M Williams**^{1,3}, **William Neale**¹, **Stacey Collister**¹, **Derek Hood**⁴, **Stefan Oscarson**⁵, **Jens Madsen**⁶, **Howard Clark**⁶, **Trevor J Greenhough**¹

¹School of Life Sciences, Keele University, Keele, United Kingdom; ²Current address: School of Biochemistry, University of Bristol, Bristol, United Kingdom; ³Current address: Bernhard Nocht Institute for Tropical Medicine, Department of Virology, Hamburg, Germany; ⁴Mammalian Genetics Unit, MRC Harwell Institute, Harwell Science and Innovation Campus, United Kingdom; ⁵School of Chemistry, University College Dublin, Dublin, Ireland; ⁶EGA Institute for Women's Health, Faculty of Population Health Sciences, University College London, London, United Kingdom

External Resource:



MS-10-1093-006_b.pdf

5:00pm - 5:20pm

Molecular basis underpinning metabolite-mediated T-cell immunity

Wael Awad¹, **Geraldine Ler**², **Jeffrey Y. W. Mak**², **Jérôme Le Nours**¹, **James McCluskey**³, **Alexandra J. Corbett**³, **David P. Fairlie**², **Jamie Rossjohn**¹

¹Department of Biochemistry and Molecular Biology, Biomedicine Discovery Institute, Monash University, Australia; ²Institute for Molecular Bioscience, The University of Queensland, Australia; ³Department of Microbiology and Immunology, Peter Doherty Institute for Infection and Immunity, University of Melbourne, Australia

External Resource:



MS-10-649-007_b.pdf

2:45pm - 5:10pm

MS-11: Ab initio powder structure analysis for polymorphism and phase transformation studies with pharmaceutical applications



Location: **Club D**
Session Chair: **Martin U. Schmidt**
Session Chair: **Fabia Gozzo**
Invited: **Kenneth Harris (UK), Jim Kaduk (USA)**

Introduction

2:45pm - 2:50pm

Introduction to session

Martin U. Schmidt, Fabia Gozzo



MS-11-1741-001.pdf

2:50pm - 3:20pm

Crystal Structures of Large-Volume Commercial Pharmaceuticals

James A Kaduk¹, Ryan L Hodge¹, Nicholas C Boaz¹, Amy M Gindhart², Thomas N Banton²

¹North Central College, Naperville, United States of America; ²ICDD, Newtown Square, United States of America;
kaduk@polycrystallography.com

External Resource: Presentation



MS-11-631-002_b.pdf

3:20pm - 3:50pm

Structure determination from powder X-ray diffraction data augmented by complementary techniques

Kenneth D. M. Harris

School of Chemistry, Cardiff University, Cardiff CF10 3AT, Wales, United Kingdom; HarrisKDM@cardiff.ac.uk

External Resource: Presentation



MS-11-1371-003_b.pdf

3:50pm - 4:10pm

Monitoring polymorphic transition of a cocrystal to a salt using time-resolved X-ray powder diffraction and solid-state nuclear magnetic resonance spectroscopy

Luzia S. Germann¹, Mihails Arhangeliskis³, Robin S. Stein¹, Robert E. Dinnebier², Tomislav Friščić¹

¹McGill University, Montreal, Canada; ²Max Planck Institute for Solid State Research, Stuttgart, Germany; ³University of Warsaw, Warsaw, Poland; luzia.germann@mail.mcgill.ca

External Resource: Presentation



MS-11-999-004_b.pdf

4:10pm - 4:30pm

Mechanism elucidation of Stepwise dehydration of pharmaceutical hydrate crystals by structure determination from powder diffraction data

Hidehiro Uekusa, Akiko Egami, Hironaga Oyama, Akiko Sekine

Department of Chemistry, Tokyo Institute of Technology, Tokyo, Japan; uekusa@chem.titech.ac.jp

External Resource: Presentation



MS-11-736-005_b.pdf

4:30pm - 4:50pm

Structure determination of racemic trichlormethiazide from powder diffraction data

Anelio Jose Dugarte Dugarte¹, Robert Toro², Jacco van de Streek³, Jose Antonio Henao², Graciela Diaz de Delgado¹, Jose Miguel Delgado¹

¹Laboratorio de Cristalografía-LNDRX, Departamento de Química, Facultad de Ciencias, Universidad de Los Andes, Merida, Venezuela, Bolivarian Republic of; ²Grupo de Investigación en Química Estructural (GIQUE), Escuela de Química, Facultad de Ciencias, Universidad Industrial de Santander, Bucaramanga, Colombia; ³Avant-garde Materials Simulation, Alte Str. 2, D-79249 Merzhausen, Germany; anelioj@gmail.com

External Resource: Presentation



MS-11-180-006_b.pdf

4:50pm - 5:10pm

Difficult structures of organic molecules and how to solve them

Marcus Müller, Dubravka Sisak Jung

DECTRIS Ltd., Baden-Daettwil, Switzerland; marcus.mueller@dectris.com

External Resource:



MS-11-592-007_b.pdf

2:45pm - 5:10pm

MS-12: Quantum crystallographic studies on intra/inter-molecular interactions



Location: **Club H**

Session Chair: **Anna Maria Makal**

Session Chair: **Chérif F. Matta**

Invited: **Jacob Overgaard** (Denmark), **Benoit Guillot** (France)

Introduction

2:45pm - 2:50pm

Introduction to session

Anna Maria Makal, **Chérif F. Matta**



MS-12-1742-001.pdf

2:50pm - 3:20pm

Beyond multipolar pseudoatom transferability: accounting for intermolecular polarization effects in protein-ligand complexes.



Theo Leduc, **Christian Jelsch**, **Benoit Guillot**

Université de Lorraine, CNRS, CRM2, F-54000 Nancy, France; benoit.guillot@univ-lorraine.fr

External Resource:



MS-12-1021-002_b.pdf

3:20pm - 3:50pm

Using advanced X-ray and neutron diffraction techniques in single molecule magnets research



Jacob Overgaard¹, **Emil Damgaard-Møller**¹, **Lennard Krause**¹, **Iurii Kibalin**², **Emil Andreassen Klahn**¹

¹Department of Chemistry, Aarhus University, Aarhus C, Denmark; ²LLB, CEA, CE de Saclay, Gif sur Yvette, 91191, France; jacobo@chem.au.dk

External Resource:



MS-12-1259-003_b.pdf

3:50pm - 4:10pm

Use of transferrable multipoles to extend the range of X-ray charge density study to variable-temperature and high pressure



Krešimir Molčanov¹, **Valentina Milašinović**¹, **Anna Krawczuk**², **Nikita Bogdanov**³, **Boris Zahkarov**³, **Elena Boldyreva**³, **Christian Jelsch**⁴

¹Rudjer Bošković Institute, Zagreb, Croatia; ²Jagiellonian University, Krakow, Poland; ³Novosibirsk State University, Novosibirsk, Russian Federation; ⁴Université de Lorraine, Nancy, France; kmolcano@irb.hr

External Resource:



MS-12-493-004_b.pdf

4:10pm - 4:30pm

NCI-ELMO: towards a more quantitative description of non-covalent interactions in macromolecules



Erna Katharina Wieduwilt¹, **Rubén Laplaza**², **Giovanni Macetti**¹, **David Arias-Olivares**², **Francesca Peccati**², **Julia Contreras-García**², **Alessandro Genoni**¹

¹CNRS & University of Lorraine, Laboratory of Theoretical Physics and Chemistry, UMR CNRS 7019, 1 Boulevard Arago, 57078 Metz, France; ²CNRS & Sorbonne University, Laboratory of Theoretical Chemistry, UMR CNRS 7616, 4 Place Jussieu, 75005 Paris, France; erna-katharina.wieduwilt@univ-lorraine.fr

External Resource:



MS-12-763-005_b.pdf

4:30pm - 4:50pm

Organic eutectics: characterization, microstructural evolution, and properties.



Titas Pramanik¹, **Ashish Anand**¹, **Janaky Sunil**², **Anjana Joseph**², **Chandrabhas Narayana**², **Somnath Dutta**³, **Tayur N. Guru Row**¹

¹Solid State & Structural Chemistry Unit, Indian Institute of Science, Bengaluru 560012, India; ²Chemistry and Physics of Materials Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Bengaluru 560064, India; ³Molecular Biophysics Unit, Indian Institute of Science, Bengaluru 560012, India.; titaspramanik1990@gmail.com

External Resource:



MS-12-410-006_b.pdf

4:50pm - 5:10pm

Strength and nature of host-guest interactions in metal-organic frameworks from a quantum chemical perspective

Michelle Ernst^{1,2}, Ganna Gryn'ova^{1,2}

¹Heidelberg Institute for Theoretical Studies (HITS gGmbH), 69118 Heidelberg, Germany; ²Interdisciplinary Center for Scientific Computing, Heidelberg University, 69120 Heidelberg, Germany; michelle.ernst@h-its.org

External Resource:



MS-12-263-007_b.pdf

2:45pm - 5:10pm

MS-13: Porous framework materials for gas adsorption/separation

Location: **Club C**

Session Chair: **Angiolina Comotti**

Session Chair: **Ryotaro Matsuda**

Invited: **Michael Zaworotko** (Ireland) , **Catharine Esterhuysen** (South Africa)

Introduction

2:45pm - 2:50pm

Introduction to session

Angiolina Comotti, Ryotaro Matsuda



MS-13-1743-001.pdf

2:50pm - 3:20pm

Crystal Engineering of Ultramicroporous Materials

Michael John Zaworotko

University of Limerick, Limerick, Ireland; xtal@ul.ie

External Resource:



MS-13-378-002_b.pdf

3:20pm - 3:50pm

The role of noncovalent interactions in the properties of porous compounds

Catharine Esterhuysen

Stellenbosch University, Stellenbosch, South Africa; ce@sun.ac.za

External Resource:



MS-13-391-003_b.pdf

3:50pm - 4:10pm

Direct observation of the xenon physisorption process in mesopores by combining in situ Anomalous Small-Angle X-ray Scattering and X-ray Absorption Spectroscopy

Armin Hoell¹, Gericke Eike^{1,2}, Wallacher Dirk¹, Wendt Robert¹, Greco Giorgia¹, Krumrey Michael³, Raoux Simone^{1,4}, Mascotto Simone⁵

¹Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany; ²Institut für Chemie, Humboldt-Universität zu Berlin, Berlin, Germany; ³Physikalisch-Technische Bundesanstalt (PTB), 10587 Berlin, Germany; ⁴Institut für Physik, Humboldt-Universität zu Berlin, Germany; ⁵Institut für Anorganische und Angewandte Chemie, Universität Hamburg, Germany.; hoell@helmholtz-berlin.de

External Resource:



MS-13-1283-004_b.pdf

4:10pm - 4:30pm

Crystal engineered hybrid ultramicroporous materials for single-step ethylene purification from C₂-CO₂ ternary mixture

Soumya Mukherjee¹, Michael J. Zaworotko²

¹Department of Chemistry, Technical University of Munich, Lichtenbergstrasse 4, 85748 Garching b. Munich, Germany; ²Bernal Institute, Department of Chemical Sciences, University of Limerick, Limerick V94 T9PX, Republic of Ireland; soumya.mukherjee@tum.de

External Resource:





MS-13-107-005_b.pdf

4:30pm - 4:50pm

Gas adsorption and separation: tuning the channel electrostatics for CO₂.

Charl Bezuidenhout, Jacopo Perego, Silvia Bracco, Piero Sozzani
University of Milano-Bicocca, Milano, Italy; charl.bezuidenhout@unimib.it

External Resource:



MS-13-767-006_b.pdf

Elucidation of CO₂ adsorption process in a bis-pyrazolate based MOF through HR-PXRD

Stephanie Terruzzi¹, Rebecca Vismara², Simona Galli², Valentina Colombo¹

¹University of Milan, Milan, Italy; ²Università degli studi dell'Insubria, Como, Italy; stephanie.terrucci@unimi.it

External Resource:



MS-13-692-007_b.pdf

MS-14: Perovskites

Location: **Terrace 2B**

Session Chair: **Chris Ling**

Session Chair: **Philip Lightfoot**

Invited: **James Rondinelli (USA)**, **Joke Hadermann (Belgium)**

Introduction

2:45pm - 2:50pm

Introduction to session

Chris Ling, **Philip Lightfoot**



MS-14-1744-001.pdf

2:50pm - 3:20pm

Uncovering hidden complexity in oxygen deficient perovskites

Maria Batuk, **Daphne Vandemeulebroucke**, **Joke Hadermann**

University of Antwerp, Antwerpen, Belgium; joke.hadermann@uantwerpen.be

External Resource:



MS-14-1198-002_b.pdf

3:20pm - 3:50pm

Understanding the thermal expansion in layered perovskite chalcogenides

James M. Rondinelli

Northwestern University, Evanston, United States of America; jrondinelli@northwestern.edu

External Resource:



MS-14-1129-003_b.pdf

3:50pm - 4:10pm

Octahedral tilting in Prussian blue analogues

Hanna L. B. Boström¹, **William R. Brant**², **Anthony E. Phillips**³

¹Max Planck Institute for Solid State Research, Germany; ²Uppsala Universitet, Sweden; ³Queen Mary University of London, UK; h.bostroem@fkf.mpg.de

External Resource:



MS-14-747-004_b.pdf

4:10pm - 4:30pm

Evidence for pressure induced 'morphotropic', octahedral tilt and 'reentrant' ferroelectric transitions in (Pb_{0.5}Bi_{0.5})(Ti_{0.5}Fe_{0.5})O₃

Pragya Singh¹, **Chandan Upadhyay**¹, **Zuzana Konôpková**², **Hanns-Peter Liermann**², **Dhananjai Pandey**¹

2:45pm - 5:10pm

External Resource:  Presentation



MS-14-515-005_b.pdf

4:30pm - 4:50pm

In situ imaging of ferroelastic domain dynamics in CsPbBr₃ perovskite nanowires by nanofocused scanning X-ray diffraction

Lucas Atila Bernardes Marcal¹, Eitan Oksenberg^{2,3}, Dmitry Dzhigaev¹, Susanna Hammarberg¹, Amnon Rothman³, Alexander Björling⁴, Eva Unger^{5,6}, Anders Mikkelsen¹, Ernesto Joselevich³, Jesper Wallentin¹

¹Synchrotron Radiation Research and NanoLund, Lund University, 22100 Lund, Sweden; ²Center for Nanophotonics, AMOLF, 1098 XG Amsterdam, Netherlands; Department of Materials; ³Interfaces, Weizmann Institute of Science, Rehovot 76100, Israel; ⁴MAX IV Laboratory, Lund University, 22100 Lund, Sweden; ⁵Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Young Investigator Group Hybrid Materials Formation and Scaling, 12489 Berlin, Germany; ⁶Division of Chemical Physics and NanoLund, Lund University, 22100 Lund, Sweden; lucas.marcal@sljus.lu.se

External Resource:  Presentation



MS-14-682-006_b.pdf

4:50pm - 5:10pm

Unraveling the mysterious intermediate state in Zr-rich PbZr_{1-x}Ti_xO₃

Nan Zhang¹, Zheyi An¹, Marek Pasiaek², Hiroko Yokota³, Mike Glazer^{4,5}, Zuo-Guang Ye⁶

¹Electronic Materials Research Laboratory, Xi'an Jiaotong University, Xi'an, China, People's Republic of; ²Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic; ³Department of Physics, Chiba University, Chiba City, Japan; ⁴Department of Physics, University of Oxford, Oxford, United Kingdom; ⁵Department of Physics, University of Warwick, Coventry, United Kingdom; ⁶Department of Chemistry and 4D LABS, Simon Fraser University, Burnaby, Canada; nzhang1@xjtu.edu.cn

External Resource:  Presentation



MS-14-765-007_b.pdf

MS-16: Pre and post publication peer review of crystallographic data

Location: **Terrace 2A**

Session Chair: **Mariusz Jaskolski**

Session Chair: **Anthony Linden**

Invited: **Stephen K. Burley (USA)**, **Brian McMahon (UK)**

Introduction

2:45pm - 2:50pm

Introduction to session

Mariusz Jaskolski, **Anthony Linden**



MS-16-1745-001.pdf

2:50pm - 3:20pm

Celebrating the 50th Anniversary of the Protein Data Bank – Prepublication Peer Review and Validation of Small-Molecule Ligands Bound to Proteins and Nucleic Acids

Stephen K. Burley

RCSB Protein Data Bank, Institute for Quantitative Biomedicine, Department of Chemistry and Chemical Biology, Rutgers Cancer Institute of New Jersey, Rutgers, The State University of New Jersey, Piscataway, NJ 08854, United States; sburley@proteomics.rutgers.edu

External Resource:  Presentation



MS-16-723-002_b.pdf

3:20pm - 3:50pm

Data scrutiny in IUCr journals

Brian McMahon

International Union of Crystallography, Chester, United Kingdom; bm@iucr.org

External Resource:  Presentation



MS-16-675-003_b.pdf

3:50pm - 4:15pm

Crystallographic review - perspectives from a chemical structural database

Suzanna Ward, Natalie Johnson, Matthew Lightfoot
The Cambridge Crystallographic Data Centre (CCDC), Cambridge, United Kingdom; ward@ccdc.cam.ac.uk

External Resource:  Presentation



MS-16-1142-004_b.pdf

4:15pm - 4:40pm

How not to publish structural results

Alexander Wlodawer

National Cancer Institute, Frederick, MD, United States of America; wlodawer@nih.gov

External Resource:  Presentation



MS-16-266-005_b.pdf

4:40pm - 5:05pm

Evolution of macromolecular model quality

Dariusz Brzezinski^{1,2,3}, Zbigniew Dauter⁴, Wlodek Minor³, Mariusz Jaskolski^{1,5}

¹Center for Biocrystallographic Research, Institute of Bioorganic Chemistry, Polish Academy of Sciences, Poznan, Poland; ²Institute of Computing Science, Poznan University of Technology, Poznan, Poland; ³Department of Molecular Physiology and Biological Physics, University of Virginia, Charlottesville, USA; ⁴Synchrotron Radiation Research Section, Macromolecular Crystallography Laboratory, National Cancer Institute, Argonne National Laboratory, Argonne, USA; ⁵Department of Crystallography, Faculty of Chemistry, A. Mickiewicz University, Poznan, Poland; dariusz.brzezinski@cs.put.poznan.pl

External Resource:  Presentation



MS-16-368-006_b.pdf

2:55pm - 5:55pm

SF-1: Software Fayre 1

Location: 221-2

Session Chair: **Martin Lutz**

<http://www.cryst.chem.uu.nl/lutz/>

2:55pm - 3:40pm

EMDA - Tools for cryoEM map validation

Rangana Sanjeeva Warshamanage

MRC Laboratory of Molecular Biology, Cambridge, United Kingdom; ranganaw@mrc-lmb.cam.ac.uk

External Resource:  Presentation

3:40pm - 4:25pm

MStruct - software for MicroStructure analysis by powder diffraction

Zdeněk Matěj¹, Milan Dopita²

¹MAX IV Laboratory, Lund University, Lund, Sweden; ²Charles University, Faculty of Mathematics and Physics, Prague;

zdenek.matej@maxiv.lu.se

External Resource:  Presentation

4:25pm - 5:10pm

Advanced tools for charge density refinement/modelling with MoProSuite

Christian Jelsch, Benoit Guillot

CRM2 CNRS Université de Lorraine, Vandoeuvre les Nancy, France; christian.jelsch@univ-lorraine.fr

5:10pm - 5:55pm

Software tools for flexibility and symmetry analysis of macromolecules

Sergei Grudin

CNRS, Grenoble, France; sergei.grudin@inria.fr

External Resource:  Presentation

MS-15: Integrative methodologies for novel thin film structures

Location: 223-4

Session Chair: **David Babonneau**

Session Chair: **Baerbel Krause**

Invited: **Jolien Dendooven (Belgium), Byeongdu Lee (USA)**

Introduction

3:45pm - 3:50pm

Introduction to session

David Babonneau, Baerbel Krause



MS-15-1727-001.pdf

3:50pm - 4:20pm

In situ study of noble metal atomic layer deposition processes using grazing incidence small angle X-ray scattering**Jolien Dendooven¹**, Eduardo Solano^{1,2}, Ji-Yu Feng¹, Ranjith K. Ramachandran¹, Matthias M. Minjaaw¹, Michiel Van Daele¹, Alessandro Coati³, Daniel Hermida-Merino⁴, Christophe Detavernier¹¹Ghent University, Dept. of Solid State Sciences, COCOON Group, Krijgslaan 281/S1, 9000 Gent, Belgium; ²ALBA Synchrotron Light Source, SWEET-NCD Beamline, Carrer de la Llum 2-26, 08290 Cerdanyola del Vallès, Spain; ³Synchrotron SOLEIL, SixS Beamline, L'Orme des Merisiers, Saint-Aubin, BP48, 91192 Gif-sur-Yvette, France; ⁴ESRF European Synchrotron, DUBBLE Beamline BM26, Avenue des Martyrs, CS40220, 38043 Grenoble, France; Jolien.Dendooven@UGent.be

External Resource:



MS-15-1002-002_b.pdf

4:20pm - 4:50pm

Symmetry-breaking in double gyroid block copolymer film**Seungyun Jo¹**, Haedong Park², Taesuk Jun¹, Kwangjin Kim², Hyunsoo Jung¹, Sungmin Park³, **Byeongdu Lee⁴**, Seungwoo Lee^{2,5}, Du Yeol Ryu¹¹Department of Chemical and Biomolecular Engineering, Yonsei University, Republic of Korea; ²KU-KIST Graduate School of Converging Science and Technology, Korea University, Republic of Korea; ³Advanced Materials Division, Korea Research Institute of Chemical Technology, Republic of Korea; ⁴Argonne National Laboratory, Lemont, United States of America; ⁵Department of Integrative Energy Engineering, Department of Biomicrosystem Technology, and KU Photonics Center, Korea University, Republic of Korea; blee@anl.gov

External Resource:



MS-15-1349-003_b.pdf

4:50pm - 5:10pm

Growth studies of thin films with total scattering in real time**Martin Roelsgaard¹**, Ann-Christin Dippel², Bo Brummerstedt Iversen¹¹Department of Chemistry & iNANO, Aarhus University, Aarhus C, Denmark; ²PETRA III, Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany; m.roelsgaard@chem.au.dk

External Resource:



MS-15-1134-004_b.pdf

5:10pm - 6:10pm

Afternoon break 1: Poster session A1, exhibition, coffee/teaLocation: **Exhibition and poster area****Poster - 01 Bioinformatics: Structural bioinformatics**Session Chair: **Jiri Cerny**

5:10pm - 6:10pm

Session Chair: **Bohdan Schneider**Session Chair: **Janusz Marek Bujnicki****Poster session abstracts****Radomír Kužel**

Poster - 01 Bioinformatics-1928-001.pdf

Exploiting new generation ab initio and homology models from databases for MR**Adam J Simpkin¹**, Jens M H Thomas¹, Ronan M Keegan², Daniel J Rigden¹¹Institute of Integrative Biology, University of Liverpool, Liverpool L69 7ZB, England; ²STFC, Rutherford Appleton Laboratory, Research Complex at Harwell, Didcot OX11 0FA, England

External Resource:



Poster - 01 Bioinformatics-1390-002_b.pdf

The analysis of CH- π interaction in protein-carbohydrate binding**Josef Houser^{1,2}**, Stanislav Kozmon^{1,3}, Deepti Mishra¹, Zuzana Hammerova², Michaela Wimmerova^{1,2,4}, Jaroslav Koca^{1,2}¹Central European Institute of Technology, Masaryk University, Kamenice 5, 625 00 Brno, Czech Republic; ²National Centre for Biomolecular Research, Masaryk University, Kamenice 5, 625 00 Brno, Czech Republic; ³Institute of Chemistry, Slovak Academy of Sciences, Dubravská cesta 9, 845 38 Bratislava, Slovak Republic; ⁴Department of Biochemistry, Faculty of Science, Masaryk University, Kotlarská 2, 611 37 Brno, Czech Republic

External Resource:



Poster - 01 Bioinformatics-989-004_b.pdf



Poster - 01 Bioinformatics-989-004_c.pdf

On the role of CO...CO interactions in the classification of beta-turns.

Consiglia Tedesco, Nancy D'Arminio, Valentina Ruggiero, Giovanni Pierri, Anna Marabotti
University of Salerno, Fisciano, Italy

External Resource:



Poster - 01 Bioinformatics-1297-005_b.pdf

Structural Characterization of missense mutation identified in BRCA2 using Comparative Biophysical and Dynamics Studies

Mudassar Ali Khan^{1,2}, Mohd. Quadir Siddiqui³, Ashok K Varma^{1,2}

¹Advanced Centre for Treatment Research and Education in Cancer, Kharghar, Navi Mumbai, India; ²Homi Bhabha National Institute, Mumbai, India; ³Alberta RNA Research and Training Institute, Department of Chemistry and Biochemistry, University of Lethbridge, 4401 University Drive, Lethbridge, AB T1K 3M4, Canada; mudassarbest@gmail.com

External Resource:



Poster - 01 Bioinformatics-742-006_b.pdf

De novo detection of symmetry in cryo-EM density maps

Michal Tykač¹, Jiří Černý¹, Garib N. Murshudov²

¹Czech Academy of Sciences, Prague, Czech Republic; ²MRC Laboratory of Molecular Biology; Michal.Tykac@ibt.cas.cz

External Resource:



Poster - 01 Bioinformatics-1290-007_b.pdf

PISACov: Expanding jsPISA with evolutionary covariance data to better determine protein quaternary state from a crystal structure

José Javier Burgos-Marmol¹, Ronan M. Keegan², Eugene Krissinel², Daniel J. Rigden¹

¹ISMIB, University of Liverpool, Liverpool, United Kingdom; ²UKRI-STFC, Rutherford Appleton Laboratory, Didcot, United Kingdom; J.J.Burgos-Marmol@liverpool.ac.uk

External Resource:



Poster - 01 Bioinformatics-823-008_b.pdf

PDBe-KB: a community-driven resource for structural and functional annotations

Mihaly Varadi, PDBe-KB Consortium

EMBL-EBI, Hinxton, United Kingdom; mvaradi@ebi.ac.uk

External Resource:



Poster - 01 Bioinformatics-911-009_b.pdf

EvoDock: Optimization of protein-ligand binding interfaces

Maximilian Edich¹, Marcel Friedrichs²

¹University of Hamburg; ²Bielefeld University; medich@PHYSnet.uni-hamburg.de

External Resource:



Poster - 01 Bioinformatics-831-010_b.pdf

Effects of mutations in the NMDA receptor GluN1 subunit on binding and dynamics: a computational approach

Zheng Chen^{1,2}, W. Bret Church¹, Karine Bastard¹, Anthony P. Duff³, Thomas Balle^{1,2}

¹Sydney Pharmacy School, Faculty of Medicine and Health, The University of Sydney, NSW 2006, Australia; ²Brain and Mind Centre, The University of Sydney, Camperdown, NSW 2050, Australia; ³Australian Nuclear Science and Technology Organisation, New Illawarra Road, Lucas Heights, NSW 2234, Australia; jake.chen@sydney.edu.au

External Resource:



Poster - 01 Bioinformatics-1600-011_b.pdf

Base pairs and their higher order structures

Małgorzata Cabaj, Paulina Dominia

Biological and Chemical Research Centre, Department of Chemistry, University of Warsaw, Poland; mkcabaj@uw.edu.pl

External Resource:



Poster - 01 Bioinformatics-1568-012_b.pdf

The rotat library: generating protein structure-specific side-chain rotamer libraries

Algirdas Grybauskas, Saulius Gražulis

Vilnius University Life Sciences Center, Saulėtekio al. 7, 10257 Vilnius, Lithuania; algirdas.grybauskas@gmc.vu.lt

External Resource:



Poster - 01 Bioinformatics-1596-013_b.pdf

Patterson positivity combined with statistical matching can estimate unobserved intensities

Anders Kadziola

University of Copenhagen, Copenhagen, Denmark



Poster - 01 Bioinformatics-1525-014_b.pdf

How the point mutation of NPC1 can affect the cholesterol transport efficiency : Molecular dynamics study

HYEJIN YOON¹, Soonmin Jang², Hyunah Jeong², Hyung Ho Lee¹

¹Seoul National University, Seoul, Korea, Republic of (South Korea); ²Sejong University, Seoul, Korea, Republic of (South Korea); yoohj@snu.ac.kr

External Resource:



Poster - 01 Bioinformatics-1416-015_b.pdf

Modeling large protein structures as graphs for automated analysis of their topology

Jan Niclas Wolf, Mariella Zunker, Jörg Ackermann, Ina Koch

Molecular Bioinformatics, Goethe-University, Frankfurt am Main, Germany; Wolf@bioinformatik.uni-frankfurt.de

External Resource:



Poster - 01 Bioinformatics-1585-016_b.pdf

Investigation of Furin inhibition to block SARS-CoV-2 spike protein cleavage and Structural stability via molecular docking and molecular dynamics simulations

Jaganathan Ramakrishnan, Archana Chinnamadh, Kumaradhas Poomani

Laboratory of Biocrystallography and Computational Molecular Biology, Department of Physics, Periyar University, Salem-636 011, India.; rjaganphy@gmail.com

External Resource:



Poster - 01 Bioinformatics-728-017_b.pdf

The first hydration layer around biomolecules is site-specific

Lada Biedermannová, Bohdan Schneider

Institute of Biotechnology, Vestec near Prague, Czech Republic

External Resource:



Poster - 01 Bioinformatics-1823-018_b.pdf

Probing Protein Structures in Solution by Molecular Dynamics Simulation and Small-Angle X-ray Scattering

Hsiao-Ching Yang¹, Shang-Wei Lin¹, Yung-Chi Ge¹, Ming-Yi Huang¹, Cheng-Han Yang¹, Wei-Min Liu¹, Anthony P. Duff², Chun-Ming Wu³, Yi-Kang Lan⁴, An-Chung Su⁴, Yi-Qi Yeh³, U-Ser Jeng^{3,4}, Pi-Tai Chou⁵

¹Department of Chemistry, Fu Jen Catholic University, Xinzhuang 24205, Taiwan; ²National Deuteration Facility, Australian Nuclear Science and Technology Organisation, Lucas Heights, NSW 2234, Australia; ³National Synchrotron Radiation Research Center, Hsinchu Science Park, Hsinchu 30076, Taiwan; ⁴Department of Chemical Engineering, National Tsing Hua University, Hsinchu 30013, Taiwan; ⁵Department of Chemistry, National Taiwan University, Taipei City 10617, Taiwan; hcyang_chem@mail.fju.edu.tw

External Resource:



Poster - 01 Bioinformatics-1861-019_b.pdf

Poster - 02 Drug design: Drug design

Session Chair: **Begoña Heras**

Session Chair: **Anton V. Zavialov**



5:10pm - 6:10pm

Poster session abstracts

Radomír Kužel



Poster - 02 Drug design-1929-001.pdf

Fragment Based Drug Discovery of SARS-CoV-2 Main Protease

Weixiao Song, Sen Li, AhWing Edith Chan, Alun Coker
University College London, London, United Kingdom

External Resource:



Poster - 02 Drug design-1215-002_b.pdf

Repurposing an ancient protein core structure: structural studies on FmtA, a novel esterase of *Staphylococcus aureus*

vikram Dalal¹, Pramod Kumar¹, Gaddy Rakhaminov², Aneela Qamar², Xin Fan², Howard Hunter², Shailly Tomar¹, Dasantila Golemi-Kotra², Pravindra Kumar¹

¹Department of Biotechnology, IIT Roorkee, Roorkee, India; ²Department of Biology, York University, 4700 Keele Street, Toronto, Canada; vdalal@bt.iitr.ac.in

External Resource:



Poster - 02 Drug design-132-003_b.pdf



Poster - 02 Drug design-132-003_c.pdf

Studies of LysSi3, a Gram-negative targeting endolysin with broad bactericidal activity.

Tatyana Prudnikova¹, Daria V Vasina², Dmitry Loginov¹, Ivana Kuta Smatanova¹

¹Laboratory of Structural Chemistry, Institute of Chemistry, Faculty of Science, University of South Bohemia in České Budějovice, Czech Republic; ²N.F. Gamaleya National Research Centre for Epidemiology and Microbiology, Ministry of Health of the Russian Federation, 123098 Moscow, Russia.

External Resource:



Poster - 02 Drug design-1163-004_b.pdf

Structural insight into the degradation selectivity of C2H2 zinc finger by thalidomide metabolite

Hirotake Furihata¹, Satoshi Yamanaka², Toshiaki Honda³, Norio Shibata³, Masaru Tanokura¹, Tatsuya Sawasaki², Takuya Miyakawa¹

¹Graduate School of Agricultural and Life Sciences, The University of Tokyo; ²Proteo-Science Center, Ehime University; ³Life Science and Applied Chemistry, Graduate School of Engineering, Nagoya Institute of Technology

External Resource:



Poster - 02 Drug design-1448-005_b.pdf

Structure determination of the motor domain of centromere associated protein E

Asuka Shibuya¹, Naohisa Ogo², Jun-ichi Sawada², Akira Asai², Hideshi Yokoyama¹

¹Faculty of Pharmaceutical Sciences, Tokyo University of Science; ²Center for Drug Discovery, Graduate School of Pharmaceutical Sciences, University of Shizuoka

External Resource:





Poster - 02 Drug design-1604-006_b.pdf

Structural studies towards the development of an oral main protease (Mpro) inhibitor to treat SARS-CoV-2 infection

Joanne Lemieux¹, Muhammad Bashir Khan¹, Arutyunova Arutyunova¹, Jimmy Lu¹, James Nieman³, D. Lorne Tyrrell², Howard S Young¹

¹Department of Biochemistry, University of Alberta, Edmonton, Canada; ²Li Ka Shing Institute of Virology, University of Alberta, Edmonton, Alberta, Canada; ³Li Ka Shing Applied Virology Institute, University of Alberta, Edmonton, Alberta, Canada,

External Resource:



Poster - 02 Drug design-1663-007_b.pdf

Poster - 03 Structure prediction: Crystal structure prediction

Session Chair: **Qiang Zhu**



5:10pm - 6:10pm

Poster session abstracts

Radomir Kužel



Poster - 03 Structure prediction-1930-001.pdf

Machine Learning on Experimental Crystal Structures to parametrize Models of the Gibbs Energy in Computational Crystallography

Detlef WM Hofmann¹, Liudmila LN Kuleshova²

¹CRS4, Pula, Italy; ²FlexCryst, Utenreuth, Germany; dwmhofmann@aol.com

External Resource:



Poster - 03 Structure prediction-758-002_b.pdf



Poster - 03 Structure prediction-758-002_c.pdf

Predicting the packing behaviour of porous organic cages

Emma Helen Wolpert, Kim E Jelfs

Department of Chemistry, Imperial College London, Molecular Sciences Research Hub, White City Campus, London, W12 0BZ, UK; e.wolpert@imperial.ac.uk

External Resource:



Poster - 03 Structure prediction-915-003_b.pdf

Come for the drug, stay for the solvent!

Ioana Sovago, Peter Wood

The Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge, CB1 2EZ, UK; isovago@ccdc.cam.ac.uk

External Resource:



Poster - 03 Structure prediction-859-004_b.pdf

Structural characterization of Cu-tpy-nucleotide ternary complexes

Suma Dilipkumar, Nethaji Munirathinam

Indian Institute of Science, Bengaluru, India; sumadilip1@gmail.com

External Resource:



Poster - 03 Structure prediction-1602-005_b.pdf

CSP: Paracetamol via Grid Search & PSO

Milan Kočí

FSNPE, Czech Technical University in Prague, Prague, Czech Republic; kocimil1@fffi.cvut.cz

External Resource:





Poster - 03 Structure prediction-1917-006_b.pdf



Poster - 03 Structure prediction-1917-006_c.pdf

5:10pm - 6:10pm

Poster - 04 Photochemistry: Solid state photo chemistry



Poster session abstracts

Radomír Kužel



Poster - 04 Photochemistry-1931-001.pdf

Combined structural and spectroscopic investigations of a series of photo- and thermoswitchable trinitrocobalt(III) coordination compounds in the solid state

Krystyna A. Deresz, Sylwia E. Kutniewska, Radosław Kamiński, Katarzyna N. Jarzemska
Chemistry Department, University of Warsaw, Warsaw, Poland; krystynaderesz@gmail.com



Poster - 04 Photochemistry-518-002_b.pdf

Structural characterization and cation distribution of Cr³⁺ substituted cobalt ferrite

M.A. Islam¹, M.Z. Ahsan², F.A. Khan¹

¹Department of Physics, Bangladesh University of Engineering and Technology, Dhaka 1000, Bangladesh; ²Departments of Chemistry and Physics, Gono Bishwabidyalay, Savar, Dhaka-1344, Bangladesh; maislam.buet.phy@gmail.com

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Poster - 04 Photochemistry-658-003_b.pdf

Strain analysis of SiNWs-GQDs core-shell heterostructures

Cosmin Romanitan, Pericle Varasteanu, Antonio Radoi, Cristina Pachiu, Iuliana Mihalache
National Institute of Microtechnologies, Bucharest, Bucharest, Romania; cosmin.romanitan@imt.ro



Poster - 04 Photochemistry-640-004_b.pdf



Poster - 04 Photochemistry-640-004_c.pdf

Resolution of ferrocene and deuterated ferrocene conformations using dynamic vibrational IR spectroscopy

Nicholas Thien Tam Tran¹, Ryan McEvey Trevorah¹, Christopher Thomas Chantler¹, Dominique Appadoo², Feng Wang³

¹School of Physics, The University of Melbourne, Parkville, Victoria 3010, Australia; ²Australian Synchrotron, 800 Blackburn Rd, Clayton Victoria 3168, Australia; ³Department of Chemistry and Biotechnology, Swinburne University of Technology, Hawthorn, Victoria 3122, Australia; nicholas2@student.unimelb.edu.au

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Poster - 04 Photochemistry-808-005_b.pdf

MBE growth Monitoring of a single GaAs nanowire by in-situ X-ray nano-diffraction

Ullrich Pietsch¹, Sayad Mohammad Mostavi Kashani¹, Jonas Vogel³, Arman Davtyan¹, Danial Bahrami¹, Ludwig Feigl², Julian Jakob², Philipp Schroth², Tilo Baumbach², Vladimir G. Dubrovskii⁴

¹University of Siegen, Siegen, Germany; ²Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany; ³University of Mainz, Germany; ⁴St. Petersburg State University, Russia; pietsch@physik.uni-siegen.de

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Poster - 04 Photochemistry-370-006_b.pdf



Poster - 04 Photochemistry-370-006_c.pdf

Controlled tuning of atomistic structure in functional materials by acoustic standing waves and electric fields

Christian Lüd¹, Elena Ovchinnikova², Anton Kulikov³, Dimitri Novikov⁴, Dirk Meyer¹, Matthias Zschornak¹

¹Institute of Experimental Physics, Technische Universität Bergakademie Freiberg, Leipziger Str. 23, 09599 Freiberg, Germany; ²Physics Department, Moscow State University, 119991 Moscow, Russia; ³A.V. Shubnikov Institute of Crystallography, FSRC "Crystallography and Photonics" RAS, Leninskiy Prospekt, 59, 119333 Moscow, Russia; ⁴Deutsches Elektronen-Synchrotron DESY, Notkestraße 85, 22607 Hamburg, Germany; christian.lued@physik.tu-freiberg.de

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Poster - 04 Photochemistry-1526-007_b.pdf

Structure and luminescent properties of $\text{KGd}_{1-x}\text{Eu}_x(\text{MoO}_4)_2$ ($0 \leq x \leq 1$)

Svetlana M. Posokhova, Dina V. Deyneko, Bogdan I. Lazoryak, Vladimir A. Morozov
Lomonosov Moscow State University, Moscow, Russian Federation; posokhovasm@gmail.com



Poster - 04 Photochemistry-488-008_b.pdf

Catalytic development and medical application of transition metal complexes (Re, Co, Cu) containing novel Salicylidene Schiff bases

Hannah van Dyk, Frederick Jacobus Francois Jacobs, Alice Brink
University of the Free State, Bloemfontein, South Africa; hannah.vandyk96@gmail.com

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Poster - 04 Photochemistry-643-009_b.pdf

Understanding small rhenium molecules kinetically and structurally in a macromolecular setting

Frederick Jacobus Francois Jacobs, Alice Brink
University of the Free State, Bloemfontein, South Africa; fjfiacobs7@gmail.com

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Poster - 04 Photochemistry-621-010_b.pdf

Excitation energy dependent tunable emission in SrZnO_2 nanophosphors

- Manju^{1,2}, Ankush Vij³, Anup Thakur¹

¹Advanced Materials Research Lab, Department of Basic and Applied Science, Punjabi University, Patiala 147 002, Punjab, India; ²Department of Physics, Punjabi University, Patiala 147 002, Punjab, India; ³Nanophosphors Lab, Department of Physics, Amity University Haryana, Gurgaon 122 413, Haryana, India; manju.rao007@gmail.com

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Poster - 04 Photochemistry-131-011_b.pdf

Photocrystallographic studies of novel nickel (II) nitro complex supplemented by IR spectroscopy and multi-temperature XRD experiments

Patryk Borowski¹, Sylwia Ewa Kutniewska¹, Radosław Kamiński¹, Adam Krówczyński¹, Dominik Schaniel², Katarzyna Natalia Jarzemska¹

¹University of Warsaw, Warsaw, Poland; ²Universite de Lorraine & CNRS, Vandoeuvre-les-Nancy, France; pz.borowski2@student.uw.edu.pl



Poster - 04 Photochemistry-440-012_b.pdf

Hybrid halobismuthates: structure and optical properties

Petr A. Buikin^{1,4}, Vitalii Yu. Kotov^{2,4}, Alexander A. Korlyukov³, Andrey B. Ilyukhin⁴

¹D. Mendeleev University of Chemical Technology of Russia, 125047, Moscow, Russian Federation; ²National Research University Higher School of Economics, 101000, Moscow, Russian Federation; ³Institute of Organoelement Compounds of RAS, 119991, Moscow, Russian Federation; ⁴N. S. Kurnakov Institute of General and Inorganic Chemistry, Russian Academy of Sciences, 119991, Moscow, Russian Federation; peterzz@mail.ru

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Poster - 04 Photochemistry-271-013_b.pdf

The Manipulation Of Metal-Metal Bonding Distances By Variation Of The Size Of N-Substituents On PNP Ligand Systems

Christo van Staden, Hendrik Gideon Visser, Marietjie Schutte-Smith
University of the Free State, Bloemfontein, South Africa; christovanstaden00@gmail.com

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Poster - 04 Photochemistry-319-014_b.pdf

5:10pm - 6:10pm

Poster - 05 MOF: Metal-organic frameworks

Session Chair: **Sergei Alexandrovich Sapchenko**

Session Chair: **Yue-Biao Zhang**



Poster session abstracts

Radomír Kužel



Poster - 05 MOF-1932-001.pdf

Kinetic and thermodynamic control in assembly of rare-earth cyamelurates

Albina Isbjakova, Vladimir Chernyshev, Viktor Tafeenko, Leonid Aslanov

Moscow State University, Leninskie Gory 1, Moscow, 119991, Russian Federation; albinabushmeleva@mail.ru

External Resource: Presentation



Poster - 05 MOF-196-002_b.pdf

High pressure, high temperature crystallography of graphite intercalation compounds

Alexandre Courac (Kurakevych)

IMPMC - Sorbonne University, Paris, France; alexandre.courac@sorbonne-universite.fr

External Resource: Presentation



Poster - 05 MOF-636-003_b.pdf

Polystyrene modification by cellulose derivative and organoclay

Lorenci Gjurgjaj¹, Enida Nushi², Altin Mele^{2,3}, Ardita Mele³, Dorina Mele³, Igli Qoshja³

¹University of Tirana, Tirana, Albania; ²Center of Techniques Studies, Ivodent Academy, Tirana, Albania; ³Department of Prosthodontics, Ivodent Academy, Tirana, Albania; lorencigjurgjaj@gmail.com

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Poster - 05 MOF-421-004_b.pdf

SYNTHESIS, STRUCTURAL STUDY, BIOLOGICAL AND NLO PROPERTIES OF THREE NEW HYBRID COMPOUNDS OF DAPSONE

Amani Hind Benahsene¹, Lamia Bendjeddou¹, Rokaya Henchiri^{2,3}, Nasreddine Ennaceur^{2,3}, Samia Zaout⁴

¹Unité de recherche de chimie de l'environnement moléculaire et structurale URCHEMS, Constantine, Algeria; ²Laboratory of Materials, Energy and Environment UR14-ES26, University of Gafsa, 2100 Gafsa, Tunisia; ³Laboratory of Quantum and Molecular Photonics, Institut d'Alembert, École normale supérieure Paris-Saclay, 94230 Cachan, France; ⁴Laboratoire d'Electrochimie des Matériaux Moléculaires et des Complexes Université Sétif 1, Algérie; amani.benahsene@hotmail.com

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Poster - 05 MOF-420-005_b.pdf

Synthesis and Characterization of ZnMgMOF-74

Juliana Assunção Pereira de Figueiredo, Gabriel Galvani, João Alves, Laise Amorim, Maximiliano Zapata, Carlos Pinheiro

Universidade Federal de Minas Gerais, 31270-901/ Belo Horizonte, MG, Brazil; japf@fis.dout.ufmg.br

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Poster - 05 MOF-558-006_b.pdf

Crystallographic Aspects of the Propanoate Salts

Jan Fábry, Erika Samolová

Institute of Physics of the Czech Academy of Sciences, Praha 8, Czech Republic; fabry@fzu.cz

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Poster - 05 MOF-1197-007_b.pdf

Kinetics in the gas adsorption process of porous coordination polymers by time-resolved X-ray powder diffraction measurement

Hirota Ashitani¹, Shogo Kawaguchi², Hiroki Ishibashi¹, Kenichi Otake³, Susumu Kitagawa³, Yoshiki Kubota¹

¹Department of Physical Science, Graduate School of Science, Osaka Prefecture University, Sakai, Osaka 599-8531, Japan; ²Japan Synchrotron Radiation Research Institute (JASRI), SPring-8, Sayo, Hyogo 679-5198, Japan; ³Institute for Integrated Cell-Material Sciences (iCeMS), Kyoto University, Kyoto 606-8501, Japan; s_h.ashitani@p.s.osakafu-u.ac.jp

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Poster - 05 MOF-1477-008_b.pdf

Multi-interactive coordination network featuring a ligand with topologically isolated p-orbitals

Yuki Wada, Hiroyoshi Ohtsu, Pavel M Usov, Masaki Kawano

Tokyo Institute of Technology, Tokyo, Japan; wada.y.am@m.titech.ac.jp

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Poster - 05 MOF-1501-009_b.pdf

Large pore isoreticular MOFs as tunable nanoreactors

Christophe M.L. Vande Velde, Rosa Fucci, Pegie Cool

University of Antwerp, Antwerpen, Belgium; christophe.vandevelde@uantwerpen.be

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Poster - 05 MOF-1528-010_b.pdf

Nalidixic acid-Ca(II) derivatives: discrete complexes and metal-organic frameworks

Vanía Andre^{1,2}, Paula C. Alves^{1,2}, Catarina Bravo^{1,2}, Juliana Mota^{1,2}

¹Centro de Química Estrutural, Instituto Superior Técnico, Universidade de Lisboa, Portugal; ²IST-ID, Lisbon, Portugal; vaniandre@tecnico.ulisboa.pt

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Poster - 05 MOF-1704-011_b.pdf

Multifunctional MOFs Based on Imidazoletricarboxylic Acid for Gas Adsorption, Sensing and Catalysis

Anantharaman Ganapathi

Indian Institute of Technology (IIT), Kanpur, India; garaman@iitk.ac.in

External Resource:



Poster - 05 MOF-1679-012_b.pdf

Fluorination and co-doping of ZIF-8 by ball mill grinding for efficient oxygen reduction electrocatalysis

Max Rautenberg^{1,2}, Marius Gernhard³, Christina Roth³, Franziska Emmerling^{1,2}

¹Federal Institute for Materials research and Testing, Berlin, Germany; ²Humboldt-Universität zu Berlin, Berlin, Germany; ³Universität Bayreuth, Bayreuth, Germany; max.rautenberg@bam.de



Poster - 05 MOF-1921-013_b.pdf

Controlling nanoparticle synthesis derived from bimetallicmetal-organic frameworks

Zhihengyu Chen¹, Zhijie Chen², Omar Farha^{2,3}, Karena W. Chapman¹

¹Department of Chemistry, Stony Brook University, Stony Brook, New York 11794, United States; ²Department of Chemistry and International Institute for Nanotechnology, Northwestern University, Evanston, Illinois 60208, United States; ³Department of Chemical and Biological Engineering, Northwestern University, Evanston, Illinois 60208, United States; zhihengyu.chen@stonybrook.edu



Poster - 05 MOF-1924-014_b.pdf

Poster - 06 Perovskites: Perovskites

Session Chair: **Philip Lightfoot**

Session Chair: **Chris Ling**



5:10pm - 6:10pm

Poster session abstracts

Radomír Kužel



Poster - 06 Perovskites-1933-001.pdf

Recognition of domain patterns using high-resolution single crystal X-ray diffraction

Semën Gorfman

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Poster - 06 Perovskites-836-002_b.pdf

Suppression mechanism of the ferroelectric polarization in multiferroic tetragonal perovskite $\text{Sr}_{1/2}\text{Ba}_{1/2}\text{MnO}_3$

Daisuke Okuyama¹, Kunihiro Yamauchi^{2,3}, Hideaki Sakai^{4,5}, Yasujiro Taguchi⁶, Yoshinori Tokura^{6,7}, Kuniyoshi Sugimoto⁸, Taku J Sato¹, Tamio Oguchi^{2,9}

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Poster - 06 Perovskites-1087-003_b.pdf

Distortion mode anomalies at $T_{\text{MIT}} = T_{\text{N}}$ in bulk PrNiO_3

Y. Maximilian Klein¹, Dariusz. J. Gawryluk¹, Tian Shang¹, Denis Sheptyakov², Vladimir Pomjakushin², Lukas Keller², Nicola Casati³, Philippe Lacorre⁴, Maria T. Fernández-Díaz⁵, Juan Rodríguez-Carvajal⁵, Marisa Medarde¹

¹Laboratory for Multiscale Materials Experiments, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland; ²Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland; ³Swiss Light Source, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland; ⁴Institut des Molécules et Matériaux du Mans (IMMM) - UMR 6283 CNRS, Le Mans Université, Avenue Olivier Messiaen, 72085 Le Mans, France; ⁵Institut Laue Langevin, 71 avenue des Martyrs, CS 20156 -38042 Grenoble CEDEX 9, France; Maximilian.Klein@psi.ch

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Poster - 06 Perovskites-1106-004_b.pdf

Thermoelastic instabilities in rare-earth perovskites REScO_3 ($\text{RE} = \text{Nd}, \text{Sm}, \text{Tb}, \text{Dy}$)

Christian Hirschle¹, Jürgen Schreuer¹, Steffen Ganschow², Isabelle Schulze-Jonack²

¹Ruhr-Universität Bochum, Bochum, Germany; ²Leibniz-Institut für Kristallzüchtung, Berlin, Germany; christian.hirschle@rub.de

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Poster - 06 Perovskites-298-005_b.pdf

Heterovalent doping of a 1D hybrid pseudo-perovskite: B site vacancy and short-range order

Candida Pipitone¹, Francesco Giannici¹, Antonino Martorana¹, Antonietta Guagliardi², Gonzalo García-Espejo³, Norberto Masciocchi³

¹Dipartimento di Fisica e Chimica "Emilio Segrè", Università di Palermo, viale delle Scienze, 90128 Palermo; ²Istituto di Cristallografia & To.Sca.Lab., Consiglio Nazionale delle Ricerche, via Valleggio 11, 22100 Como, Italy; ³Dipartimento di Scienza e Alta Tecnologia & To.Sca.Lab., Università dell'Insubria, via Valleggio 11, 22100 Como, Italy; candida.pipitone@unipa.it

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Poster - 06 Perovskites-1233-006_b.pdf

Structure of the RNiO_3 single crystals ($R = \text{Nd}, \text{Sm}, \text{Gd}, \text{Dy}, \text{Y}, \text{Ho}, \text{Er}, \text{Lu}$)

Dariusz Jakub Gawryluk¹, Yannick Maximilian Klein¹, Mirosław Kozłowski², Philippe Lacorre³, Anthony Linden⁴, Marisa Medarde¹

¹Paul Scherrer Institut, Villigen PSI, Switzerland; ²Łukasiewicz Research Network Tele & Radio Research Institute, Warsaw, Poland; ³Institut des Molécules et Matériaux du Mans (IMMM) - UMR 6283 CNRS, Le Mans Université, Le Mans, France; ⁴Department of Chemistry, University of Zürich, Zürich, Switzerland; dariusz.gawryluk@psi.ch

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Poster - 06 Perovskites-1162-007_b.pdf

The magnetic-structural relationships of $[\text{CuX}_6]^{4-}$ [$\text{X} = \text{Cl}^-$ or Br^-] perovskites containing n -carboxyalkylammonium cations of various chain lengths

Shalene Natalia Bothma¹, Mark. M Turnbull², Belinda van der Westhuizen¹, Christopher. P Landee³, Charles Sheppard⁴, Liezel Van der Merwe¹, Fan Xiao^{5,6}, Melanie Rademeyer¹

¹Department of Chemistry, University of Pretoria, Pretoria, South Africa; ²Carlson School of Chemistry and Biochemistry, Clark University, 950 Main St., Worcester, Massachusetts, 01610, USA; ³Department of Physics, Clark University, 950 Main St., Worcester, Massachusetts, 01610, USA; ⁴Cr Research group, Department of Physics, University of Johannesburg, Auckland Park, Johannesburg, 2006, South Africa; ⁵Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland; ⁶Department of Chemistry and Biochemistry, University of Bern, Freiestrasse 3, Bern, Switzerland; shalenebothma@gmail.com

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Poster - 06 Perovskites-486-008_b.pdf

Halide Perovskites – structural systematisation and what we learn from it.

Joachim Breternitz^{1,2}, Susan Schorr^{1,3}

¹Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany; ²Universität Potsdam, Potsdam, Germany; ³Freie Universität Berlin, Berlin, Germany; joachim.breternitz@helmholtz-berlin.de

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Poster - 06 Perovskites-923-009_b.pdf

Stoichiometric molecular hydration of interstitial sites in a close-packed ionic lattice

Chris Ling¹, Frederick Marlon¹, Alex Brown¹, Andrey Maljuk², Bernd Büchner², William Lewis¹, Matthew Sale¹, Ian Luck¹

¹The University of Sydney, Sydney, Australia; ²IFW-Dresden, Dresden, Germany; chris.ling@sydney.edu.au

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Poster - 06 Perovskites-739-010_b.pdf

Effect of Bi non-stoichiometry on the crystallographic structure of Na_{1/2}Bi_{1/2}TiO₃

Ahmed Gadelmawla¹, Kevin Riess¹, Manuel Hinterstein², Kyle Webber¹, Neamul Khansur¹

¹Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany; ²Karlsruher Institut für Technologie, Karlsruhe, Germany; ahmed.gadelmawla@fau.de

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Poster - 06 Perovskites-655-011_b.pdf

Synthesis, Structure and Simulation of magnetic disorder of doped Copper manganite La_{0.65}Ce_{0.05}Sr_{0.3}Mn_{1-x}Cu_xO₃

MAROUAN OUMEZZINE

University of Monastir, Monastir, Tunisia; oumezzine@hotmail.co.uk

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Poster - 06 Perovskites-347-012_b.pdf

Fascinating structure and physical properties of lead-free hybrid perovskites for multifunctional applications

Seham Kamal Abdel-Aal¹, Ahmed Sabry Abdel-Rahman¹, Gabor Bortel², Arron Pekker², Katalin Kamaras², Gyula Faigel²

¹Cairo University, Giza, Egypt; ²Wigner Research Centre for Physics, Hungarian Academy of Sciences; seham@sci.cu.edu.eg

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Poster - 06 Perovskites-350-013_b.pdf

Crystal structure of SrCo_{1-x}Mo_xO_{3-δ} (0 ≤ x ≤ 1) perovskites obtained under oxidizing and reducing conditions with potential use as electrodes for intermediate-temperature symmetrical solid-oxide fuel cells

Stefania Orozco Gil^{1,2}, Ana Laura Larralde², Susana Adelina Larrondo^{1,3}, Diego Germán Lamas²

¹UNIDEF-MINDEF-CONICET, Departamento de Investigaciones en Sólidos, CITEDEF; ²ITECA-ECYT-UNSAM-CONICET, Laboratorio de Cristalografía Aplicada; ³Instituto de Investigación e Ingeniería Ambiental, 3iA-UNSAM; sgil@citedef.gob.ar

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Poster - 06 Perovskites-729-014_b.pdf

Incommensurate structures of $\text{Pb}(\text{Zr},\text{Sn})\text{O}_3$

Marek Paściak¹, Irena Jankowska-Sumara², Maria Podgórna², Andrzej Majchrowski³, Miloš Kopecký¹, Jiří Kub¹

¹Institute of Physics of the Czech Academy of Sciences, Prague 8, Czech Republic; ²Institute of Physics, Pedagogical University, ul. Podchorążych 2, Kraków, Poland; ³Institute of Applied Physics, Military University of Technology, ul. Gen. Witolda Urbanowicza 2, 00-908 Warsaw, Poland; pasciak@fzu.cz

External Resource: Presentation



Poster - 06 Perovskites-1305-015_b.pdf

Experimental Electron Density Distribution and QTAIM Topological Analysis for the Perovskite Mineral: *Sulphohalite* – $\text{Na}_6(\text{SO}_4)_2\text{FCl}$

Agata Wróbel, Roman Gajda, Krzysztof Woźniak

¹Department of Chemistry, Biological and Chemical Research Centre, University of Warsaw, Poland; am.wrobel2@student.uw.edu.pl

External Resource: Presentation



Poster - 06 Perovskites-1364-016_b.pdf

Why the knowledge of the anharmonicity is important for the structural processes that govern the orthorhombic/tetragonal phase transformation in chlorine-substituted MAPbI_3

Götz Schuck¹, Daniel M. Többsen¹, Tong Sy Tien², Susan Schorr^{1,3}

¹Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany; ²University of Fire Prevention and Fighting, Vietnam; ³Freie Universität Berlin, Germany; goetz.schuck@helmholtz-berlin.de

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Poster - 06 Perovskites-1546-017_b.pdf

In situ structure characterization of perovskite-based catalysts

Simone Gallus, Eko Budiyo, Claudia Weidenthaler

Max-Planck-Institut für Kohlenforschung, Kaiser-Wilhelm-Platz 1, 45470 Mülheim an der Ruhr, Germany; gallus@mpi-muelheim.mpg.de

External Resource: Presentation



Poster - 06 Perovskites-1587-018_b.pdf

Pulsed-laser deposition of LuFeO_3 – an in-situ x-ray diffraction study

Václav Holý¹, Lukáš Horák¹, Sondas Bauer², Adriana Rodrigues², Berkin Nergis², Tilo Baumbach²

¹Charles University, Praha, Czech Republic; ²Karlsruhe Institute of Technology, Karlsruhe, Germany; holy@mag.mff.cuni.cz

External Resource: Presentation



Poster - 06 Perovskites-1677-019_b.pdf

5:10pm - 6:10pm

Poster - 07 Powder: Powder diffraction - general, structure refinement



Poster session abstracts

Radomír Kužel



Poster - 07 Powder-1934-001.pdf

Use of intermolecular distances from ssNMR in crystal structure determination from powder diffraction data

Jan Rohlíček¹, Libor Kobera², Michal Hušák³, Jiří Brus²

¹Institute of Physics of the Czech Academy of Sciences, Na Slovance 2, Prague 8, 182 21, Czech Republic; ²Institute of Macromolecular Chemistry, Czech Academy of Sciences, Heyrovsky Square 2, Prague, 16206, Czech Republic; ³Department of Solid State Chemistry, University of Chemical Technology Prague, Prague 6, 166 28, Czech Republic; rohlicek@fzu.cz

External Resource: Presentation



Poster - 07 Powder-1354-002_b.pdf

Structure determination of soft crystal polymorphs by using prediction technique with powder X-ray diffraction data

Shigeaki Obata¹, Hitoshi Goto^{1,2}

¹CONFLEX Corporation, Tokyo, Japan; ²Information and Media Center, Toyohashi University of Technology, Toyohashi, Japan; obata@conflex.co.jp

External Resource:



Poster - 07 Powder-1518-003_b.pdf

Easy Automation & More Accurate Analysis with HighScore(Plus) V4.

Thomas Degen, Egbert Bron, Mustapha Sadki

Malvern Panalytical B.V., Almelo, Netherlands, The; thomas.degen@panalytical.com

External Resource:



Poster - 07 Powder-600-004_b.pdf



Poster - 07 Powder-600-004_c.pdf

Structural characterization of $Mg_xCo_{3-x}P_2O_8$ solid solutions

Maria Angeles Tena², Rafael Mendoza¹, Camino Trobajo¹, José R. García¹, Santiago Garcia-Granda¹

¹University of Oviedo, Oviedo, Spain; ²Jaume I University, Castellon, Spain; tena@uji.es

External Resource:



Poster - 07 Powder-800-005_b.pdf

5:10pm - 6:10pm

Poster - 08 General: General interest



Poster session abstracts

Radomir Kužel



Poster - 08 General-1936-001.pdf

Ducks in space groups! Students grasping 3D-arrangement of symmetry elements with hands-on models

Nico Graw, Dietmar Stalke

Institut für Anorganische Chemie, Georg-August-Universität Göttingen, 37077 Göttingen, Germany; ngraw@chemie.uni-goettingen.de

External Resource:



Poster - 08 General-749-002_b.pdf

Helping researchers to solve their structures: automation and user guidance in CCP4 Cloud

Oleg Kovalevskiy, Andrey Lebedev, Eugene Krissinel

CCP4, Rutherford Appleton Laboratory, UKRI STFC, Didcot, United Kingdom; oleg.kovalevskiy@stfc.ac.uk

External Resource:



Poster - 08 General-1482-003_b.pdf

The Argentinian Crystal Growing Contest and other educational activities in Argentina during the COVID-19 pandemic

Sebastián Klinke^{1,2}, Valeria Cintia Fuertes^{1,3}, Vanina Gisela Franco^{1,4}, Clarisa Ester Alvarez^{1,5}, Diego Germán Lamas^{1,6}

¹Argentinian Association of Crystallography (AACr); ²Fundación Instituto Leloir, IIBBA-CONICET, Ciudad Autónoma de Buenos Aires, Argentina; ³INFIQC, UNC-CONICET, Facultad de Ciencias Químicas, Córdoba Capital, Pcia. de Córdoba, Argentina; ⁴Instituto de Física del Litoral, UNL-CONICET, Santa Fe Capital, Pcia. de Santa Fe, Argentina; ⁵Centro de Estudios Fotosintéticos y Bioquímicos-CONICET, FBioyF-UNR, Rosario, Pcia. de Santa Fe, Argentina; ⁶ITECA, UNSAM-CONICET, ECyT, Laboratorio de Cristalografía Aplicada, San Martín, Pcia. de Buenos Aires, Argentina; dlamas@unsam.edu.ar

External Resource:





Poster - 08 General-1552-004_b.pdf

Alarm sounded for lack of bringing and building crystallography in Ethiopia

Alebel Nibret Belay

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Poster - 08 General-392-005_b.pdf



Poster - 08 General-392-005_c.pdf

AsCA 2022 - 17th Conference of the Asian Crystallographic Association in Korea

Kyeong Kyu Kim, Sangho Lee, Changsuk Oh

Sungkyunkwan University, Suwon, Korea, Republic of (South Korea); kyeongkyu@skku.edu

External Resource:



Poster - 08 General-1388-006_b.pdf

University remote teaching in crystal chemistry during the COVID-19 pandemic: positive and negative aspects

Olga V. Grineva

Chemistry Department of Moscow M. V. Lomonosov State University, Moscow, Russia; ovg@phys.chem.msu.ru

External Resource:



Poster - 08 General-1715-007_b.pdf

5:10pm - 6:10pm

Workshop - High Score: Easy automation and more accurate analysis with High Score Plus (V4)

Location: virtual

Website - virtual

6:10pm - 7:00pm

KN-4: Crystal forms in pharmaceutical applications

Location: Terrace 2B

Session Chair: **Marijana Đaković**

Susan Reutzel-Edens

Crystal forms in pharmaceutical applications: Olanzapine, a gift to crystal chemistry that keeps on giving

Susan Reutzel-Edens¹, Rajni Bhardwaj²

¹Cambridge Crystallographic Data Centre, Cambridge, United Kingdom; ²AbbVie, North Chicago, IL USA; sreutzel-edens@ccdc.cam.ac.uk

External Resource:



KN-4-1607-001_b.pdf

6:10pm - 7:00pm

KN-5: State of the art understanding of diffraction from aperiodic crystals

Location: Terrace 2A

Session Chair: **Ma. Louise Antonette Navarro De Las Peñas**

Uwe Grimm

Diffraction from aperiodic crystals: the state of the art

Uwe Grimm

The Open University, Milton Keynes, United Kingdom; uwe.grimm@open.ac.uk

External Resource:



KN-5-1182-001_b.pdf

6:10pm - 7:00pm

KN-6: The Coronavirus Structural Task Force

Location: Club A

Session Chair: **Marcin Nowotny**

Andrea Thorn

The Coronavirus Structural Task Force

Andrea Thorn

Universität Hamburg, Germany; andrea.thorn@uni-hamburg.de

External Resource:



KN-6-1222-001_b.pdf

7:15pm - 10:15pm	IUCr: IUCr assembly Location: Club H Session Chair: Sven Lidin Session Chair: Alex Ashcroft Session Chair: Luc Van Meervelt IUCr assembly 1 Videos: Finance report - Part 2	-
Date: Monday, 16/Aug/2021		
9:00am - 9:50am	KN-7: Electron crystallography of molecular crystals Location: Terrace 2A Session Chair: Václav Petříček Lukáš Palatinus Electron crystallography of molecular crystal Lukáš Palatinus Institute of Physics of the CAS, Prague, Czech Republic; palat@fzu.cz External Resource:  Presentation	+
	KN-8: Order and disorder in metal-ion battery materials Location: Terrace 2B Session Chair: Radovan Cerny Artem Abakumov Order and disorder in metal-ion battery materials Artem Abakumov Skolkovo Institute of Science and Technology, Moscow, Russian Federation; a.abakumov@skoltech.ru External Resource:  Presentation	+ +
9:00am - 9:50am	KN-9: Crystalline sponge, metal-organic assemblies Location: Club A Session Chair: Masaki Kawano Makoto Fujita Crystalline Sponge Method: Recent Updates and Applications Makoto Fujita The University of Tokyo, School of Engineering, Tokyo, Japan; mfujita@appchem.t.u-tokyo.ac.jp External Resource:  Presentation	+
9:50am - 10:20am	Morning break 2: Exhibition, posters, coffee/tea Location: Exhibition and poster area	+
10:20am - 12:45pm	MS-17: Automation in bio-crystallography: tools, perspectives and applications Location: Club A Session Chair: Santosh Panjikar Session Chair: Melanie Vollmar Invited: Katherine McAuley (UK), Jose Marquez (France) Introduction 10:20am - 10:25am Introduction to session Santosh Panjikar, Melanie Vollmar  MS-17-1746-001.pdf	+ +
	10:25am - 10:55am Online Crystallography: Automated, Remote Controlled Protein-to-Structure Pipelines for Drug Design Jose Antonio Marquez European Molecular Biology Laboratory, Grenoble, France External Resource:  Presentation  MS-17-1179-002_b.pdf	+

Automated data collection at the Swiss Light Source macromolecular crystallography beamlines

Katherine Evelyn McAuley, Chia-Ying Huang, Jakub Kaminski, Nathalie Anna Meier, Ezequiel Panepucci, May Elizabeth Sharpe, Kate Mary Louise Smith, Laura Franceline Sin Ae Vera, Justyna Aleksandra Wojdyla
Paul Scherrer Institut, Villigen, Switzerland

External Resource:



MS-17-1445-003_b.pdf

11:25am - 11:45am

Fully automated data collection and remote access in macromolecular crystallography beamlines at the Photon Factory, Japan

Yusuke Yamada^{1,2}, **Akira Shinoda**¹, **Naohiro Matsugaki**^{1,2}, **Masahide Hikita**^{1,2}, **Masahiko Hiraki**^{2,3}, **Toshiya Senda**^{1,2}

¹Structural Biology Research Center, Institute of Materials Structure Science, High Energy Accelerator Research Organization, 1-1 Oho, Tsukuba, Ibaraki, Japan; ²School of High Energy Accelerator Science, The Graduate University for Advanced Studies, 1-1 Oho, Tsukuba, Ibaraki, Japan; ³Mechanical Engineering Center, Applied Research Laboratory, High Energy Accelerator Research Organization, 1-1 Oho, Tsukuba, Ibaraki, Japan

External Resource:



MS-17-1542-004_b.pdf

11:45am - 12:05pm

Millisecond Time-Resolved Crystallography using Film Mixing and Plunge Cooling

Matthew Jordan McLeod¹, **Jonathan Clinger**¹, **David Moreau**¹, **Todd Holyoak**², **Robert Thorne**¹

¹Cornell University, Ithaca NY, United States of America; ²University of Waterloo, Waterloo ON, Canada; mjm758@cornell.edu

External Resource:



MS-17-1245-005_b.pdf

12:05pm - 12:25pm

Automated ML-based sample centering for macromolecular X-ray crystallography with MXAimbot

Isak Lindhé, **Zdenek Matej**, **Gustavo Lima**, **Jie Nan**, **Mikel Egurian**, **Ana Gonzales**, **Elmir Jagudin**, **Oskar Aurelius**, **Jonathan Schurmann**, **Jörn Janneck**

MAX IV Laboratory, Lund, Sweden; isak.lindhe@maxiv.lu.se

External Resource:



MS-17-1067-006_b.pdf

12:25pm - 12:45pm

xia2.multiplex: a multi-crystal data analysis pipeline

Richard James Gildea, **James Beilsten-Edmands**, **Danny Axford**, **Sam Horrell**, **Robin Leslie Owen**, **Graeme Winter**
Diamond Light Source Ltd, Oxfordshire, United Kingdom; richard.gildea@diamond.ac.uk

External Resource:



MS-17-1260-007_b.pdf

MS-18a: Phase transitions in complex materials (structure and magnetism) I

Location: **Terrace 2B**

Session Chair: **Yuichi Shimakawa**

Session Chair: **Alexandra Gibbs**

Invited: **Midori Amano Patino** (Japan), **Patrick Woodward** (USA)

Introduction

10:20am - 10:25am

Introduction to session

Yuichi Shimakawa, **Alexandra Gibbs**



MS-18a-1747-001.pdf

10:25am - 10:55am

Phase Transitions in Hybrid Layered Halide Perovskites – Hydrogen Bonding Meets Octahedral Tilting

Patrick Woodward, **Noah Holzapfel**, **Tianyu Liu**, **Joseph Race**, **Alexander Milder**
Ohio State University, Columbus, United States of America; woodward.55@osu.edu

External Resource:



10:20am - 12:45pm



MS-18a-1623-002_b.pdf

10:55am - 11:25am

Complex A-site magnetism in quadruple perovskite materials

Midori Amano Patino¹, Fabio Denis Romero^{1,2}, Masato Goto¹, Takashi Saito³, Fabio Orlandi⁴, Pascal Manuel⁴, Attila Szabo^{4,5}, Paul Attfield⁶, Yuichi Shimakawa¹

¹ICR, Kyoto University, JP; ²Hakubi Center for Advanced Research, Kyoto University, JP; ³Institute of Materials Structure Science, KEK, JP; ⁴ISIS Neutron and Muon Source, UK; ⁵Department of Physics, University of Oxford, UK; ⁶CSEC, The University of Edinburgh, UK; amano.midori@stefani.3e@kyoto-u.ac.jp

External Resource:



MS-18a-769-003_b.pdf

11:25am - 11:45am

Charge order-disorder crossover and Co-O bond anomalies in the Co₃O₂BO₃ ludwigite

Carlos William Galdino¹, Daniele Freitas², Lais Rabello², Chyntia Contreras Medrano², Maximiliano Zapata⁷, Carlos B. Pinheiro⁷, Gustavo de Medeiros Azevedo⁶, Rodolfo Tartaglia¹, Alberto Rodríguez-Velamazán⁵, G. Garbarino³, M. Núñez-Reguero⁶, Eduardo Granado¹

¹Gleb Wataghin Institute of Physics, University of Campinas (UNICAMP), Campinas, São Paulo, 13083-859, Brazil; ²Institute of Physics, University of Campinas (UNICAMP); ³Instituto de Física, Universidade Federal Fluminense, Campus da Praia Vermelha, Niterói, RJ, 24210-346, Brazil; ⁴European Synchrotron Radiation Facility, 38043 Grenoble, France; ⁵Instituto de Física, Universidade Federal do Rio Grande do Sul (UFRGS), Porto Alegre, RS, 90040-060, Brazil; ⁶Institut Laue Langevin, 38042 Grenoble, France; ⁷Institut Néel / CNRS-UJF, 38042 Grenoble, France; ⁸Departamento de Física, Universidade Federal de Minas Gerais, Belo Horizonte, MG, 31270-901, Brazil; galdino@ifi.unicamp.br

External Resource:



MS-18a-563-004_b.pdf

11:45am - 12:05pm

Competition between spin-orbit coupling and molecular orbital crystal in pyrochlore ruthenate In₂Ru₂O₇

Aleksandra Krajewska^{1,2}, Tomohiro Takayama^{2,3}, Alexander Yaresko², Jürgen Nuss², Alexandra Gibbs^{1,2,4}, Sebastian Bette², Hidenori Takagi^{2,3,5}

¹ISIS Neutron and Muon Source, Didcot, United Kingdom; ²Max Planck Institute for Solid State Research, Stuttgart, Germany; ³Institute for Functional Matter and Quantum Technologies, University of Stuttgart, Stuttgart, Germany; ⁴School of Chemistry, University of St Andrews, St Andrews, United Kingdom; ⁵Department of Physics, University of Tokyo, Tokyo, Japan; aleksandra.krajewska@stfc.ac.uk

External Resource:



MS-18a-1120-005_b.pdf

12:05pm - 12:25pm

Cation order and magnetic behaviour in mixed metal bismuth scheelite Bi₃FeMo₂O₁₂

Matilde Saura-Muzquiz¹, Frederik Marlton¹, Bryce Mullens¹, Jiatu Liu¹, Thomas Vogt², Helen Maynard-Casely³, Maxim Avdeev³, Brendan Kennedy¹

¹School of Chemistry, University of Sydney, Sydney, NSW 2006, Australia; ²Department of Chemistry & Biochemistry, University of South Carolina, 1212 Greene Street, Columbia, SC 29208; ³Australian Centre for Neutron Scattering, ANSTO, New Illawarra Road, Lucas Heights NSW 2234, Australia; matilde.saura@sydney.edu.au

External Resource:



MS-18a-1024-006_b.pdf

12:25pm - 12:45pm

Correlated disorder-to-order crossover in the local structure of K_xFe_{2-y}Se_{2-z}S_z superconductor

Emil Bozin¹, Robert Koch¹, Panagiotis Mangelis², Hechang Lei¹, Reinhard Neder³, Marshall McDonnell⁴, Mikhail Feygenson⁴, Cedimir Petrovic¹, Alexandros Lappas²

¹Brookhaven National Laboratory, Upton, NY, United States of America; ²IESL FORTH, Heraklion, Greece; ³University of Erlangen-Nuremberg, Erlangen, Germany; ⁴Oak Ridge National Laboratory, Oak Ridge, TN, United States; bozin@bnl.gov

External Resource:



MS-18a-881-007_b.pdf

10:20am - 12:45pm

MS-19: Crystal structures of pharmaceutical and organic compounds from electron diffraction

Location: **Terrace 2A**

Session Chair: **Ute Kolb**

Session Chair: **Petr Brázda**

Invited: **Enrico Mugnaioli (Italy)**, **Brent Nannenga (USA)**

Introduction

10:20am - 10:25am

Introduction to session

Ute Kolb, **Petr Brázda**



MS-19-1748-001.pdf

10:25am - 10:55am

Combining MicroED and GIWAXS for determining structure and orientation of organic semiconductor thin films

Brent Nannenga

Arizona State University, Tempe, United States of America; brent.nannenga@asu.edu

External Resource:



MS-19-1186-002_b.pdf

10:55am - 11:25am

Strategies for structure solution of small-molecule organics by 3D ED using a small beam

Enrico Mugnaioli¹, **Iryna Andrusenko**¹, **Mauro Gemmi**¹, **Partha P. Das**², **Athanassios Galanis**², **Stavros Nicolopoulos**²

¹Center for Nanotechnology Innovation@NEST, Istituto Italiano di Tecnologia, Piazza San Silvestro 12, Pisa 56127, Italy;

²NanoMEGAS SPRL, Rue Émile Claus 49 bte 9, Brussels1050, Belgium; Enrico.Mugnaioli@iit.it

External Resource:



MS-19-927-003_b.pdf

11:25am - 11:45am

The crystal structure determination of an organic dye with triclinic symmetry by electron diffraction

Sergi Plana Ruiz^{1,2}, **Yasar Krysiak**³, **Joaquim Portillo Serra**⁴, **Edith Alig**⁵, **Sònia Estradé**¹, **Francesca Peiró**¹, **Ute Kolb**^{2,6}

¹LENS, MIND/IN2UB, University of Barcelona, Barcelona, Catalonia; ²Institut für Angewandte Geowissenschaften, Technische Universität Darmstadt, Darmstadt, Germany; ³Fyzikální Ústav, Akademie věd České Republiky, Prague, Czech Republic; ⁴NanoMegs SPRL, Brussels, Belgium; ⁵Institut für Anorganische Chemie und Analytische Chemie, Goethe-Universität Frankfurt, Frankfurt, Germany; ⁶Institut für Anorganische Chemie und Analytische Chemie, Johannes Gutenberg-Universität Mainz, Mainz, Germany; sergiplana@hotmail.com

External Resource:



MS-19-388-004_b.pdf

11:45am - 12:05pm

Refinement with multipolar scattering factors

Barbara Gruza, **Michał Leszek Chodkiewicz**, **Paulina Maria Dominiak**

Biological and Chemical Research Centre, Department of Chemistry, University of Warsaw, Poland; b.gruza@uw.edu.pl

External Resource:



MS-19-259-005_b.pdf

12:05pm - 12:25pm

Improving data quality for 3D electron diffraction (3DED) by Gatan Image Filter

Taimin Yang, **Hongyi Xu**, **Xiaodong Zou**

Stockholm University, Stockholm, Sweden; taimin.yang@mmk.su.se

External Resource:



MS-19-662-006_b.pdf

12:25pm - 12:45pm

3D electron diffraction: a dedicated device for structural elucidation of nanocrystalline particles

Gustavo Santiso-Quinones, **Eric Hovestreydt**, **Arianna E. Lanza**, **Gunther Steinfeld**

ELDICO Scientific AG, 5234 Villigen, Switzerland; santiso@eldico.ch

External Resource:



MS-19-815-007_b.pdf

MS-20: Dynamic frameworks

Location: **Club C**

Session Chair: **Christopher SUMBY**

Session Chair: **Michael John Zaworotko**

Invited: **Hoi Ri Moon** (Republic of Korea), **Yao Chen** (China)

Introduction

10:20am - 10:25am

Introduction to session

Christopher Sumby, Michael John Zaworotko



MS-20-1749-001.pdf

10:25am - 10:55am

Flexible Metal-Organic Frameworks for Hydrogen Isotope Separation

Hoi Ri Moon

Department of Chemistry, Ulsan National Institute of Science and Technology, Ulsan, Korea, Republic of (South Korea);

hoirimoon@unist.ac.kr

External Resource:



MS-20-1194-002_b.pdf

10:55am - 11:25am

Novel composite platform: Biomolecules-incorporation for biocatalysis, separation and biopharmaceutical formulations

Yao Chen

Nankai University, Tianjin, China, People's Republic of; chenyao@nankai.edu.cn

External Resource:



MS-20-1379-003_b.pdf

11:25am - 11:45am

Dynamic frameworks: the role of non-covalent interactions

Susan Ann Bourne

University of Cape Town, Cape Town, South Africa; susan.bourne@uct.ac.za

External Resource:



MS-20-830-004_b.pdf

11:45am - 12:05pm

Synthesis and structural properties of isostructural Zn(II) M₁₂L₈ poly-[n]-catenane using the 2,4,6-tris(4-pyridyl)benzene (TPB) ligand

Javier Marti-Rujas, Stefano Torresi, Antonino Famulari

Politecnico di Milano, Milan, Italy; javier.marti@polimi.it

External Resource:



MS-20-777-005_b.pdf

12:05pm - 12:25pm

Cocrystallization, high pressure/low temperature behaviour and vapochromism in a family of aurophilic copper-gold supramolecular networks.

Emanuele Priola¹, Nadia Curetti², Domenica Marabello¹, Jacopo Andreo³, Alessia Giordana¹, Lorenza Operti¹, Piera Benna², Eliano Diana¹

¹Department of Chemistry, Università di Torino, Via Pietro Giuria 7, 10125 Torino, Italy; ²Department of Earth sciences, University of Torino, Via Valperga Caluso 35, 10125, Turin, Italy; ³Dipartimento di Scienze Chimiche, della Vita e della Sostenibilità Ambientale, Università di Parma, Viale G. P. Usberti 17A, 43100 Parma, Italy; emanuele.priola@unito.it

External Resource:





MS-20-574-006_b.pdf

12:25pm - 12:45pm

Structural modifications occurring during the water sorption processes on a potential material for autonomous indoor humidity control

Patrice Kenfack Tsohngang¹, Thierry Yannick Sakam Nchedoung¹, Dominik Fröhlich², Emrah Hastürk³, Florence Porcher⁴, Christoph Janiak³

¹University of Dschang, Department of Chemistry, PO Box 67, Dschang, Cameroon; ²Fraunhofer-Institut for Solar Energy Systems ISE, Division Thermal Systems and Buildings, Heidenhofstraße 2, 79110 Freiburg, Germany; ³Institut für Anorganische Chemie und Strukturchemie, Heinrich-Heine-Universität Düsseldorf, Universitätsstraße 1, 40225 Düsseldorf, Germany; ⁴Laboratoire Léon Brillouin (LLB), UMR 12 CEA/CNRS, Bât. 563 CEA Saclay, 91191 Gif-sur-Yvette cedex, France; pakenfack@gmail.com

External Resource:



MS-20-502-007_b.pdf

MS-21: Structure, modeling and properties of quasicrystals

Location: **Club B**

Session Chair: **Michael Engel**

Session Chair: **Cesar Baban Pay Gómez**

Invited: **Tsunemoto Yamada (Japan), Priya Subramanian (UK)**

Introduction

10:20am - 10:25am

Introduction to session

Michael Engel, Cesar Baban Pay Gómez



MS-21-1750-001.pdf

10:25am - 10:55am

Atomic structures of Tsai-type icosahedral quasicrystals and approximants

Tsunetomo Yamada

Tokyo University of Science, Tokyo, Japan; tsunetomo.yamada@rs.tus.ac.jp

External Resource:



MS-21-1413-002_b.pdf

10:55am - 11:25am

How to determine thermodynamically stable soft matter quasicrystals efficiently?

Priya Subramanian¹, Daniel Ratliff², Alastair Rucklidge³, Andrew Archer⁴

¹Mathematical Institute, University of Oxford, Oxford OX2 6GG, United Kingdom; ²Department of Mathematics, Physics and Electrical Engineering, Northumbria University, Newcastle upon Tyne NE1 8ST, United Kingdom; ³School of Mathematics, University of Leeds, Leeds LS2 9JT, United Kingdom; ⁴Department of Mathematical Sciences and Interdisciplinary Centre for Mathematical Modelling, Loughborough University, Loughborough LE11 3TU, United Kingdom; priya.subramanian@maths.ox.ac.uk

External Resource:



MS-21-1634-003_b.pdf

11:25am - 11:45am

The d-AICuRh stability – the proof of the random-tiling hypothesis by the distribution moments analysis

ireneusz Jozef Buganski, Radoslaw Strzalka, Janusz Wolny

AGH University of Science and Technology, Krakow, Poland; ireneusz.buganski@fis.agh.edu.pl

External Resource:



MS-21-947-004_b.pdf

11:45am - 12:05pm

Beyond Golay-Rudin-Shapiro

Shelomo Ishaq Ben-Abraham

Ben-Gurion University of the Negev, Beer Sheba, Israel; shelomo.benabraham@gmail.com

External Resource:





MS-21-157-005_b.pdf

12:05pm - 12:25pm

Molecular dynamics simulation of complex alloy structures

JungWen Yeh¹, Kouji Tomita², Yuuta Imanari², Masaya Uchida^{1,3}

¹Department of Information Systems, Graduate School of Engineering, Saitama Institute of Technology; ²Department of Information Systems, Faculty of Engineering, Saitama Institute of Technology; ³Advanced Science Research Laboratory, Saitama Institute of Technology; f0010dug@sit.ac.jp

External Resource:



MS-21-1250-006_b.pdf

12:25pm - 12:45pm

Atomic resolution holography for characterizing the local structure in quasicrystals

Jens R. Stellhorn¹, Shinya Hosokawa², Koji Kimura³, Kouichi Hayashi³, Natalie Boudet⁴, Nils Blanc⁴, Gilbert Chahine⁴, Marc de Boissieu⁵

¹Dept. of Applied Chemistry, Hiroshima University, Higashi-Hiroshima 739-8527, Japan; ²Dept. of Physics, Kumamoto University, Kumamoto 860-8555, Japan; ³Dept. of Physical Science and Engineering, Nagoya Institute of Technology, Aichi 466-8555, Japan; ⁴Univ. Grenoble Alpes, CNRS, Institut Néel, Grenoble 38042, France; ⁵Univ. Grenoble Alpes, CNRS, SIMaP, Grenoble F-38000, France; stellhoj@hiroshima-u.ac.jp

External Resource:



MS-21-908-007_b.pdf

MS-22: Methods and software developments for magnetic-structure analysis

Location: 223-4

Session Chair: J. Manuel Perez-Mato

Invited: Juan Rodriguez-Carvajal (Spain), Václav Petříček (Czech Republic)

Introduction

10:20am - 10:25am

Introduction to session

Juan Manuel Perez-Mato



MS-22-1751-001.pdf

10:25am - 10:55am

Jana2020 - Magnetic option

Václav Petříček, Margarida Henriques, Michal Dušek

Institute of Physics, ASCR, Praha, Czech Republic; petricek@fzu.cz

External Resource:



MS-22-1041-002_b.pdf

10:55am - 11:25am

Developments in FullProf for magnetic structures determination in superspace

Juan Rodriguez-Carvajal

Institut Laue-Langevin, Grenoble, France; jrc@ill.eu

External Resource:



MS-22-1188-003_b.pdf

11:25am - 11:45am

MagStREXS: a crystallographic software for magnetic structure determination through resonant X-ray magnetic diffraction data

Pablo J. Bereciartua¹, Juan Rodriguez-Carvajal², Sonia Francoual¹

¹Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany; ²Institut Laue-Langevin (ILL), Grenoble, France; pablo.bereciartua@desy.de

External Resource:



MS-22-955-004_b.pdf

10:20am - 12:45pm

11:45am - 12:05pm

Asphericity of magnetisation density and anisotropy in rare-earth pyrochlores via polarized neutron diffraction and iterative entropy maximization

Iurii Andreevich Kibalin, Arsen Gukasov

LLB, CEA Saclay, Gif-sur-Yvette, France; iurii.kibalin@cea.fr

External Resource:



MS-22-782-005_b.pdf

12:05pm - 12:25pm

Magnetic x-ray standing waves

Michał Kamiński, Heiko Schulz-Ritter, Martin Tolkiehn

Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany; michal.kaminski@desy.de

External Resource:



MS-22-1128-006_b.pdf

12:25pm - 12:45pm

Global optimization of magnetic structure analysis by semidefinite relaxation method

Ryoko Oishi-Tomiyasu¹, Keisuke Tomiyasu², Masato Hagihara³

¹Kyushu University, 744 Moto'oka, Nishi-Ward, Fukuoka, Japan; ²NISSAN ARC Ltd., 1 Natsushima-cho, Yokosuka, Kanagawa, Japan;

³High Energy Accelerator Research Organization, 203-1 Shirakata, Tokai, Naka, Ibaraki, Japan; tomiyasu@imi.kyushu-u.ac.jp

External Resource:



MS-22-1236-007_b.pdf

MS-23: Ptychography: present and near future

Location: **Club D**

Session Chair: **Manuel Guizar Sicaïros**

Session Chair: **Julio Cesar da Silva**

Invited: **Chris Jacobsen (USA), Julian Reinhardt (USA)**

Introduction

10:20am - 10:25am

Introduction to session

Manuel Guizar Sicaïros, Julio Cesar da Silva



MS-23-1752-001.pdf

10:25am - 10:55am

Ptychography: how it has developed, and where it might lead

Chris Jacobsen

Argonne Lab/Northwestern University, Argonne, United States of America; cjacobsen@anl.gov



MS-23-1391-002_b.pdf

10:55am - 11:25am

Collaborative software solutions and data standards for ptychographic imaging

Juliane Reinhardt¹, Dylan McReynolds¹, Harinarayan Krishnan^{1,2}, David Shapiro¹, Bjoern Enders³, Pete Jemian⁴, Daniel Ching⁴, Junjing Deng⁴, Tekin Bicer⁴, Nicholas Schwarz⁴, Andi Barbour⁵, Wen Hu⁵, Daniel Allan⁵, Dmitri Gavrilov⁵, Alexander Hexemer¹

¹Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, United States; ²Center for Advanced Mathematics for Energy Research Applications (CAMERA), Lawrence Berkeley National Laboratory, Berkeley, CA 94720, United States; ³National Energy Research Scientific Computing Center (NERSC) Lawrence Berkeley National Laboratory, Berkeley, CA 94720, United States; ⁴Advanced Photon Source, Argonne National Laboratory, Lemont, IL 60439, United States; ⁵National Synchrotron Light Source II, Brookhaven National Laboratory, Upton, NY 11973, United States; jreinhardt@lbl.gov

External Resource:



MS-23-1395-003_b.pdf

11:25am - 11:45am

Quantitative analysis of cementitious materials by X-ray ptychographic nanotomography

S. Shirani¹, A. Cuesta¹, A. G. De La Torre¹, J.C. Da Silva², D. Karpov³, A. Diaz⁴, M. Holler⁴, P. Trtik⁴, M. A.G. Aranda¹

¹Universidad de Malaga, Malaga, Spain; ²Universite Grenoble Alpes, Grenoble, France; ³ESRF synchrotron, Grenoble, France; ⁴Paul Scherrer Institut, Villigen, Switzerland; shiva_shirani@uma.es

10:20am - 12:45pm

External Resource:



MS-23-748-004_b.pdf

11:45am - 12:05pm

Imaging of synapses in 3D with non-destructive synchrotron X-ray ptychography

Carles Bosch¹, Ana Diaz², Alexandra Pacureanu³, Mirko Holler², Elisabeth Müller⁴, Andreas Schaefer¹

¹The Francis Crick Institute, London, United Kingdom; ²cSAXS beamline, Paul Scherrer Institut, Villigen, Switzerland; ³ID16A beamline, ESRF, Grenoble, France; ⁴Electron Microscopy Facility, Paul Scherrer Institut, Villigen, Switzerland; carles.bosch@crick.ac.uk

External Resource:



MS-23-1121-005_b.pdf

12:05pm - 12:25pm

Spectral X-ray ptychography for the investigation of technical catalysts

Anico Kulow¹, Samy Ould-Chick², Redhouane Boudjehem¹, Jean Louis Hazemann¹, Tuiana Shoinkhorova², Alla Dikhtiarenko², Mohammed A. Alabdullah², Jorge Gascon², Rachid Sougrat³, Julio César da Silva¹

¹Univ. Grenoble Alpes, CNRS, Grenoble INP, Institut Néel, 38000 Grenoble, France; ²King Abdullah University of Science and Technology, KAUST Catalysis Center, Advanced Functional Materials, Thuwal 23955, Saudi Arabia; ³King Abdullah University of Science and Technology, Core Labs, Thuwal 23955, Saudi Arabia; anico.kulow@neel.cnrs.fr

External Resource:



MS-23-1140-006_b.pdf

12:25pm - 12:45pm

Coupled ptychography and tomography reconstruction of experimental data

Maik Kahnt^{1,2}, Johannes Becher³, Dennis Brückner^{1,2}, Yakub Fam³, Thomas L. Sheppard^{3,4}, Tobias Weissenberger⁵, Felix Wittwer^{1,2}, Jan-Dierk Grunwaldt^{3,4}, Wilhelm Schwieger⁵, Christian G. Schroer^{1,2}

¹Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany; ²Department Physik, Universität Hamburg, Hamburg, Germany; ³Institute for Chemical Technology and Polymer Chemistry, Karlsruhe Institute of Technology, Karlsruhe, Germany; ⁴Institute of Catalysis Research and Technology, Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, Germany; ⁵Institute of Chemical Reaction Engineering, Friedrich-Alexander-University Erlangen-Nürnberg, Erlangen, Germany; maik.kahnt@maxiv.lu.se

External Resource:



MS-23-1097-007_b.pdf

MS-24: Data-driven discovery in crystallography

Location: **Club H**

Session Chair: **Olivier C. Gagné**

Session Chair: **Anton Oliynyk**

Invited: **Wenhao Sun (USA)**, **Aria Mansouri Tehrani (Switzerland)**

Introduction

10:20am - 10:25am

Introduction to session

Olivier C. Gagné, **Anton Oliynyk**



MS-24-1753-001.pdf

10:25am - 10:55am

Unsupervised Knowledge Discovery in 'Big' Materials Data

Wenhao Sun

University of Michigan, Ann Arbor, United States of America; wsun@umich.edu

External Resource:



MS-24-603-002_b.pdf

10:55am - 11:25am

Predicting ground state and metastable crystal structures using elemental and phonon mode

Aria Mansouri Tehrani, Bastien F. Grosso, Ramon Frey, Nicola A. Spaldin

ETH Zurich, Zurich, Switzerland; aria.mansouri.t@mat.ethz.ch

External Resource:



10:20am - 12:45pm



MS-24-1351-003_b.pdf

11:25am - 11:45am

Beyond the constraints of chemistry: Crystal structure discovery in particle simulations

Julia Dshemuchadse^{1,2}, Pablo F. Damasceno^{1,3}, Carolyn L. Phillips⁴, Sharon C. Glotzer¹, **Michael Engel**^{1,5}

¹University of Michigan, Ann Arbor, MI, USA; ²Cornell University, Ithaca, NY, USA; ³University of California, San Francisco, CA, USA; ⁴Argonne National Laboratory, Argonne, IL, USA; ⁵Friedrich-Alexander University Erlangen-Nürnberg, Erlangen, Germany; michael.engel@fau.de

External Resource:



MS-24-857-004_b.pdf

11:45am - 12:05pm

Data-driven approaches on pair distribution function data: matrix factorization and clustering

Shuyan Zhang, Jie Gong, B. Reeja Jayan, Alan J. H. McGaughey

Carnegie Mellon University, Pittsburgh, United States of America; szhang2@andrew.cmu.edu

External Resource:



MS-24-894-005_b.pdf

12:05pm - 12:25pm

First-principle diffraction simulations as a tool to solve the nanodiffraction problem

Hande Öztürk¹, I. Cevdet Noyan²

¹Ozyegin University, Istanbul, TURKEY; ²Columbia University, New York, USA; hande.ozturk@ozyegin.edu.tr

External Resource:



MS-24-128-006_b.pdf

12:25pm - 12:45pm

Study of noncovalent interactions using crystal structure data in the Cambridge Structural Database

Milan Milovanović¹, Jelena Živković¹, Dragan Ninković¹, Jelena Blagojević Filipović¹, Dubravka Vojislavljević-Vasilev¹, Ivana Veljković², Ivana Stanković², Dušan Malenov³, Vesna Medaković³, Dušan Veljković³, **Snežana Zarić**³

¹Innovation center of the Faculty of Chemistry, Belgrade, Serbia; ²Institute of Chemistry, Technology and Metallurgy, University of Belgrade, Belgrade, Serbia; ³Faculty of Chemistry, Belgrade University, Belgrade, Serbia; szaric@chem.bg.ac.rs



MS-24-1139-007_b.pdf

SF-2: Software Fayre 2

Location: 221-2

Session Chair: Martin Lutz

<http://www.cryst.chem.uu.nl/lutz/>

10:20am - 11:05am

Using next generation ab initio models with AMPLE

Adam James Simpkin

University of Liverpool, Liverpool, United Kingdom; hasimpk@liverpool.ac.uk

External Resource:



11:05am - 11:50am

What literature papers are related to my diffraction dataset? Pydatarecognition - a web project of the IUCr Journals and Columbia University

Martin Karlsen¹, Berrak Ozer¹, Peter Raymond Strickland², Simon Westrip², Nicola Ashcroft², Brian McMahon², David Holden², Song Sang Koh², **Simon J. L. Billinge**¹

¹Columbia University, New York, USA; ²International Union of Crystallography, Chester, United Kingdom; sb2896@columbia.edu

External Resource:



11:50am - 12:35pm

SIMBAD: Sequence independent MR

Adam James Simpkin

University of Liverpool, Liverpool, United Kingdom; hasimpk@liverpool.ac.uk

External Resource:



10:20am - 12:45pm



12:45pm - 2:45pm	Lunch 2: Exhibition, posters, lunches Location: Exhibition and poster area Meeting ECA1: ECA Council Meeting Location: Club H	⊕
12:45pm - 2:45pm	Session Chair: Udo Heinemann Session Chair: Arie van der Lee ECA council meeting 1 CS-2: Commercial session: Xenocs Location: Terrace 2A Session Chair: Jerome Boutant Session Chair: Milan Dopita 30 min company presentation video CS-3: Why Spot-Cap® is the best option for protein purification (Chromotek) Location: Terrace 2A Session Chair: Milan Dopita 30 min company presentation Video	⊕
1:30pm - 2:00pm	MS-25: Structural biology against coronavirus/covid-1 Location: Club A Session Chair: Sarah EJ Bowman Session Chair: Lu Zhang Session Chair: Gianluca Santoni Invited: Xuhui Huang (China) Introduction	⊕
2:00pm - 2:30pm	2:45pm - 2:50pm Introduction to session <u>Sarah Bowman, Lu Zhang, Gianluca Santoni</u>	⊕
2:45pm - 5:10pm		



MS-25-1754-001.pdf

2:50pm - 3:20pm

Millisecond Functional Dynamics of RNA Polymerases Elucidated by Markov State Models

Xuhui Huang
 The Hong Kong University of Science and Technology, Kowloon, Hong Kong S.A.R. (China); xuhuihuang@ust.hk

External Resource: Presentation

MS-25-1361-002_b.pdf

3:20pm - 3:40pm

Co-crystallization of hepatitis C virus NS3/4A inhibitors and SARS-CoV-2 main protease using high density acoustic droplet ejection (ADE)

Babak Andj^{1,3}, Dale F. Kreitler¹, Desigan Kumaran^{2,3}, Alexei S. Soares¹, Jantana Keereetawee², Jean Jakoncic¹, Wuxian Shi¹, Martin R. Fuchs¹, John Shanklin², Sean McSweeney^{1,2,3}

¹Center for BioMolecular Structure, NSLS-II, Brookhaven National Laboratory, Upton, NY 11973-5000, United States; ²Biology Department, Brookhaven National Laboratory, Upton, NY 11973-5000, United States; ³National Virtual Biotechnology Laboratory (NVBL), US Department of Energy, Washington, DC, United States

External Resource: Presentation

MS-25-1204-003_b.pdf

3:40pm - 4:00pm

Structural basis of mRNA cap modification by SARS-CoV-2: Role of metal ions and implications for COVID-19 severity by emerging variants

Thiruselvam Viswanathan¹, Anurag Misra¹, Shailee Arya¹, Siu-Hong Chan², Shan Qi¹, Nan Dai², Luis Martinez-Sobrido³, Yogesh Gupta¹

¹University of Texas Health at San Antonio, San Antonio, USA; ²New England Biolabs, Ipswich, USA; ³Texas Biomedical Research Institute, San Antonio, USA

External Resource: Presentation

MS-25-1229-004_b.pdf

4:00pm - 4:20pm

Crystallographic fragment screening of SARS-CoV-2 drug discovery targets

Daren Fearon^{1,2}, Alice Douangamath^{1,2}, Ailsa Powell^{1,2}, Alex Dias^{1,2}, Anthony Aimon^{1,2}, Jose Brandao-Neto^{1,2}, Louise Dunnett^{1,2}, Rachael Skyner^{1,2}, Tyler Gorrie-Stone^{1,2}, Warren Thompson^{1,2}, Frank von Delft^{1,2,3,4}

¹Diamond Light Source Ltd, Didcot, United Kingdom; ²Research Complex at Harwell, Harwell Science and Innovation Campus, Didcot, OX11 0FA, UK; ³Centre for Medicines Discovery, University of Oxford, Old Road Campus, Roosevelt Drive, Headington, OX3 7DQ,

UK; ⁴Department of Biochemistry, University of Johannesburg, Auckland Park, 2006, South Africa

External Resource:



MS-25-1266-005_b.pdf

4:20pm - 4:40pm

A structure-guided, taxonomic-based approach to the design of broad-spectrum coronavirus protease inhibitors

Andrew D Mesecar, Sarah E St. John, Emma K Lendy, Brandon J Anson, Mackenzie E Chapman, Arun K Ghosh
Purdue University, W Lafayette, United States of America

External Resource:



MS-25-1195-006_b.pdf

4:40pm - 5:00pm

Structure of SARS-CoV-2 papain-like protease PLpro reveals a framework for antiviral inhibitor design

Vasundara Srinivasan¹, Nadine Werner¹, Sven Falke¹, Hevilla Brognaro¹, Sebastian Guenther², Patrick Reinke², Atia-tul-Wahab³, Iqbal Choudhary³, Alke Meents², Christian Betzel^{1,4}

¹Universität Hamburg, Department of Chemistry, Institute of Biochemistry and Molecular Biology and Laboratory for Structural Biology of Infection and Inflammation, c/o DESY, 22607 Hamburg, Germany.; ²Center for Free-Electron Laser Science, DESY, Notkestrasse 85, 22607 Hamburg, Germany.; ³Dr. Panjwani Center for Molecular Medicine and Drug Research International Center for Chemical and Biological Sciences (ICCBS), University of Karachi, Karachi-75270, Pakistan.; ⁴Hamburg Centre for Ultrafast Imaging (CUI), Universität Hamburg, Luruper Chaussee 149, 22761, Hamburg, Germany.

External Resource:



MS-25-1321-007_b.pdf

MS-26: Solution scattering and combined techniques for biological systems, including component dynamics

Location: **Club B**

Session Chair: **Frank Gabel**

Session Chair: **Masaaki Sugiyama**

Invited: **Mitsunori Ikeguchi** (Japan), **Anne Martel** (France)

Introduction

2:45pm - 2:50pm

Introduction to session

Frank Gabel, **Masaaki Sugiyama**



MS-26-1755-001.pdf

2:50pm - 3:20pm

Motion of a Membrane Enzyme as Seen by SANS

Waqas Javed^{1,2,3}, **Christine Ebel**¹, **Cedric Orelle**², **Jean-Michel Jault**², **Anne Martel**³

¹IBS; Univ. Grenoble Alpes, CNRS, CEA; Grenoble, 38000; France; ²Molecular Microbiology & Structural Biochemistry (MMSB) UMR 5086; CNRS/University of Lyon; Lyon, 69000; France; ³Institut Laue Langevin, Grenoble, France; martela@ill.fr

External Resource:



MS-26-907-002_b.pdf

3:20pm - 3:50pm

MD-SAXS: Hybrid method of molecular dynamics simulations and small-angle x-ray scattering experiments

Mitsunori Ikeguchi^{1,2}

¹Yokohama City University, Yokohama, Japan; ²RIKEN, Center for Computational Science, Yokohama, Japan; ike@tsurumi.yokohama-cu.ac.jp

External Resource:



MS-26-983-003_b.pdf

3:50pm - 4:10pm

Transient complexes of the Nsp7, Nsp8 and Nsp12 in SARS-CoV-2 replication transcription complex

Greg Hura

Lawrence Berkeley National Laboratory, Berkeley, United States of America

2:45pm - 5:10pm

External Resource:



MS-26-1172-004_b.pdf

4:10pm - 4:30pm

The dynamics and interactions of Scs proteins from *Proteus mirabilis*

Andrew Whitten¹, Furlong Emily², Choudhury Hassanul², Kurth Fabian², Duff Anthony¹, Martin Jennifer²

¹Australian Nuclear Science and Technology Organisation, Lucas Heights, Australia; ²Institute for Molecular Bioscience, University of Queensland, Australia

External Resource:



MS-26-1025-005_b.pdf

4:30pm - 4:50pm

Application of a lanthanide tag for evaluation of conformational states of a multidomain protein

Tomohide Saio¹, Hiroshi Nakagawa², Soya Hiramatsu³, Mizue Asada⁴, Honoka Kawamukai^{1,3}, Toshikazu Nakamura⁴, Koichiro Ishimori^{3,5}

¹Institute of Advanced Medical Sciences, Tokushima University, Tokushima, Japan; ²Materials Sciences Research Center, Japan Atomic Energy Agency, Tokai, Japan; ³Graduate School of Chemical Sciences and Engineering, Hokkaido University, Sapporo, Japan; ⁴Instrument Center, Institute for Molecular Science, Okazaki, Japan; ⁵Department of Chemistry, Faculty of Science, Hokkaido University, Sapporo, Japan; saio@tokushima-u.ac.jp

External Resource:



MS-26-981-006_b.pdf

4:50pm - 5:10pm

An Objective Metric to Guide Background Correction and Interpretation of Small Angle X-ray Scattering Data

Yunyun Gao^{1,2}, Timothy R. Stachowski³, Edward H. Snell³, Thomas D. Grant³, Arwen R. Pearson¹

¹Institute of Nanostructure and Solid State Physics, Universität Hamburg, Hamburg, Germany; ²The Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany; ³Hauptman-Woodward Medical Research Institute, Buffalo, NY, USA

External Resource:



MS-26-1029-007_b.pdf

MS-27: New trends in pharmaceutical materials

Location: **Club D**

Session Chair: **Nikoletta B. Bathori**

Session Chair: **Laszlo Fabian**

Invited: **Tonglei Li (USA)**, **Doris Braun (Austria)**

Introduction

2:45pm - 2:50pm

Introduction to session

Nikoletta B. Bathori, **Laszlo Fabian**



MS-27-1756-001.pdf

2:50pm - 3:20pm

Troublesome hydrates of alkaloids

Doris E. Braun

University of Innsbruck, Innsbruck, Austria; doris.braun@uibk.ac.at

External Resource:



MS-27-846-002_b.pdf

3:20pm - 3:50pm

Kinetic Retraction at the Onset of Concomitant Crystallization

Tonglei Li

Purdue University, West Lafayette, United States of America; tonglei@purdue.edu

External Resource:





MS-27-1573-003_b.pdf

3:50pm - 4:10pm

"Particle Informatics": Evolving methods for understanding particle properties

Andrew Gerrard Patrick Maloney, Alexandru Aurelian Moldovan, Murray George Read
Cambridge Crystallographic Data Centre, Cambridge, United Kingdom; maloney@ccdc.cam.ac.uk

External Resource:



MS-27-842-004_b.pdf

4:10pm - 4:30pm

A Novel Physics-based Ensemble Modeling Approach that Utilizes Crystal Packing to Predict Aqueous Thermodynamic Solubility

Rajni Miglani Bhardwaj, Richard Hong, Nathan Abraham, Alessandra Mattel, Ahmad Sheikh
Solid-State Chemistry, Abbvie, North Chicago, United States of America; rajni.bhardwaj@abbvie.com

External Resource:



MS-27-930-005_b.pdf

4:30pm - 4:50pm

The harvesting of small molecule structure and dynamic data for macromolecular and catalytic usage.

Alice Brink
University of the Free State, Bloemfontein, South Africa; brinka@ufs.ac.za

External Resource:



MS-27-822-006_b.pdf

4:50pm - 5:10pm

Absolute configuration directly determined from 3D electron diffraction data

Paul Benjamin Klar¹, Petr Brázda¹, Yasar Krysiak^{1,2}, Mariana Klementová¹, Lukas Palatinus¹
¹Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic; ²Institute of Inorganic Chemistry, Leibniz University Hannover, Hannover, Germany; paul.klar@fzu.cz

External Resource:



MS-27-1113-007_b.pdf

MS-28: Theory and practice of supramolecular synthons in crystal engineering

Location: **Club C**

Session Chair: **Seiji Tsuzuki**

Session Chair: **Alessia Bacchi**

Invited: **Jindrich Fanfrlik** (Czech Republic), **Berta Gomez-Lor** (Spain)

Introduction

2:45pm - 2:50pm

Introduction to session

Seiji Tsuzuki, **Alessia Bacchi**



MS-28-1757-001.pdf

2:50pm - 3:20pm

Modulation of halogen, chalcogen and pnictogen bonds by σ -hole tuning

Jindrich Fanfrlik
Institute of Organic Chemistry and Biochemistry of the CAS, Prague, Czech Republic; fanfrlik@uochb.cas.cz

External Resource:



MS-28-1146-002_b.pdf

3:20pm - 3:50pm

Benzothiadiazole-based luminescent stimuli-responsive materials: The role of "2S-2N" square synthon on their supramolecular arrangement and switchable behaviour

Berta Gómez-Lor, **Marcelo Echeverri**

2:45pm - 5:10pm

External Resource:



MS-28-1160-003_b.pdf

3:50pm - 4:10pm

Combining modified CCDC tools to predict multicomponent formation: co-crystals of nevirapine and benzoic derivatives

Rogeria Nunes Costa¹, Duane Choquesillo-Lazarte², Elna Pidcock³, Silvia Lucia Cuffini¹, Lourdes Infantes⁴

¹Instituto de Ciência e Tecnologia, Universidade Federal de São Paulo, 12231-280 São José dos Campos, Brazil; ²Laboratorio de Estudios Cristalográficos, Instituto Andaluz de Ciencias de la Tierra, CSIC, 18100 Armilla, Granada, Spain; ³Cambridge Crystallographic Data Centre, Cambridge, CB2 1EZ, United Kingdom; ⁴Instituto de Química y Física Rocasolano, CSIS, 28006 Madrid, Spain; rogeria.ncosta@gmail.com

External Resource:



MS-28-719-004_b.pdf

4:10pm - 4:30pm

Gold(III) as an effective electrophilic site, namely coinage bond donor: assembly of AuCl₄⁻ units into supramolecular anionic polymers

Giuseppe Resnati¹, Andrea Daolio¹, Andrea Pizzi¹, Giancarlo Terraneo¹, Maurizio Ursini¹, Antonio Frontera²

¹Politecnico di Milano, Milano, Italy; ²Universitat de les Illes Balears, Palma de Mallorca (Balears), Spain; giuseppe.resnati@polimi.it

External Resource:



MS-28-724-005_b.pdf

4:30pm - 4:50pm

Experimental and *ab initio* molecular dynamics study of hydrogen bond systems in selected crystals

Leszek M. Malec, Mateusz Z. Brela, Katarzyna M. Stadnicka

Faculty of Chemistry of Jagiellonian University in Kraków, Gronostajowa 2, 30-387 Kraków, Poland; malec@chemia.uj.edu.pl

External Resource:



MS-28-275-006_b.pdf

4:50pm - 5:10pm

Thermally Actuating Multifunctional Molecular Crystals

Durga Prasad Karothu¹, Rodrigo Ferreira¹, Luca Catalano¹, Ghada Dushaq², Mahmoud Rasras², Panče Naumov¹

¹Department of chemistry, New York University Abu Dhabi, Abu Dhabi, United Arab Emirates; ²Department of Electrical and Computer Engineering, New York University Abu Dhabi, Abu Dhabi, United Arab Emirates; dpk3@nyu.edu

External Resource:



MS-28-569-007_b.pdf

MS-29: Texture, strain and structure in metals and ceramics

Location: 223-4

Session Chair: David Rafaja

Invited: Efthymios Polatidis (Switzerland), Jana Šmilauerová (Czech Republic)

Introduction

2:45pm - 2:50pm

Introduction to session

David Rafaja



MS-29-1758-001.pdf

2:50pm - 3:20pm

Tailoring the TRIP effect of austenitic stainless steels with selective laser melting

Efthymios Polatidis¹, Christos Sofras¹, Capek Jan¹, Ariyan Arabi-Hashemi², Christian Leinenbach², Markus Strobl¹

¹Paul Scherrer Institute, Villigen PSI, Switzerland; ²Empa – Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland; efthymios.polatidis@psi.ch

External Resource:





MS-29-1257-002_b.pdf

3:20pm - 3:50pm

Phase transformation pathway in Ti-15Mo studied by in situ synchrotron x-ray diffraction

Pavel Zháňal, Jana Šmilauerová, Petr Hrcuba, Lukáš Horák, Václav Holý
Charles University, Prague, Czech Republic; jana.smlauerova@gmail.com

External Resource:



MS-29-586-003_b.pdf

3:50pm - 4:10pm

Microsecond time resolved X-ray diffraction for the fast determination of fatigue behavior beyond one billion cycles

Doriana Vinci, Vincent Jacquemain, Christophe Cheuleu, Vincent Michel, Olivier Castelnau, Veronique Favier, Nicolas Ranc
Laboratoire PIMM, Arts et Métiers Institute of Technology, CNRS, HESAM Université, Paris, France; doriana.vinci@ensam.eu

External Resource:



MS-29-587-004_b.pdf

4:10pm - 4:30pm

Mechanisms of elastic-plastic deformation in magnesium alloy studied using neutron diffraction and crystallite group method

Przemysław Kot¹, Andrzej Baczański¹, Marcin Wroński¹, Sebastian Wroński¹, Christian Scheffzük², Gizo Bokuchava², Vadim Sikolenko²

¹AGH University of Science and Technology, Faculty of Physics and Applied Computer Science, Kraków, Poland; ²Joint Institute for Nuclear Research, Frank Laboratory of Neutron Physics, Joliot-Curie 6, Dubna 141980, Russia; Przemyslaw.Kot@fis.agh.edu.pl

External Resource:



MS-29-1358-005_b.pdf

4:30pm - 4:50pm

Texture and eco-piezoceramics

Luis E. Fuentes-Cobas¹, Juan R. Narváez-Monroy¹, Alejandro Campos-Rodríguez¹, María E. Montero-Cabrera¹, Rodrigo Domínguez-García¹, Edgar E. Villalobos-Portillo², Luis Fuentes-Montero³, Benjamín Batista-Fierro⁴, Marcela S. Luévano-Jáquez⁴, Lorena Pardo⁵

¹Centro de Investigación en Materiales Avanzados, S.C., Chihuahua, Mexico; ²European Synchrotron Radiation Facility, Grenoble, France; ³Diamond Light Source, Didcot, UK; ⁴Universidad Autónoma de Chihuahua, Chih., México; ⁵Instituto de Ciencia de Materiales de Madrid, Madrid, Spain; luis.fuentes@cimav.edu.mx

External Resource:



MS-29-1223-006_b.pdf

4:50pm - 5:10pm

Superhardness in boron carbide through nanostructuring

Fernando Igoa^{1,2}, Simon Delacroix^{1,2}, Yang Song¹, Yann Le Godec², Cristina Coelho-Diogo³, Christel Gervais¹, Gwenaëlle Rousse⁴, David Portehault¹

¹Sorbonne Université, CNRS, Laboratoire de Chimie de la Matière Condensée de Paris (LCMCP), Paris, France.; ²Sorbonne Université, CNRS, Institut de Minéralogie, Physique des Matériaux et Cosmochimie (IMPMC), Paris, France.; ³Sorbonne Université, CNRS, Institut des Matériaux de Paris Centre (IMPC), Paris, France.; ⁴Sorbonne Université, Collège de France, CNRS, Chimie du Solide et de l'Energie (CSE), Paris, France.; fernando.igoa_saldana@upmc.fr

External Resource:



MS-29-912-007_b.pdf

MS-30: Magnetic structures of novel and functional materials

Location: Club H

Session Chair: Virginie Simonet

Session Chair: Václav Petříček

Invited: Wei Tian (USA), Jonathan White (Switzerland)

Introduction

2:45pm - 2:50pm

Introduction to session

Virginie Simonet, Václav Petříček

2:45pm - 5:10pm



MS-30-1759-001.pdf

2:50pm - 3:20pm

Investigating the nature of the magnetoelectric coupling in molecular $(\text{ND}_4)_2[\text{FeCl}_5(\text{D}_2\text{O})]$ via neutron scattering studies**W. Tian, R. S. Fishman, H. B. Cao, G. Sala, D. M. Pajerowski, V. O. Garlea, T. Hong, L. L. Daemen, Y. Q. Cheng, J. A. Fernandez-Baca**Oak Ridge National Laboratory, Oak Ridge, United States of America; wtf6@ornl.gov

MS-30-179-002_b.pdf

3:20pm - 3:50pm

Multi-k magnetic phases and topological charges in the candidate Weyl semimetal CeAlGe **Jonathan White**Paul Scherrer Institute, Villigen, Switzerland; jonathan.white@psi.ch

External Resource:



MS-30-1176-003_b.pdf

3:50pm - 4:10pm

Novel incommensurate magnetic phase in the magnetoelectric Sr-doped cobaltate $\text{CaBaCo}_4\text{O}_7$ **Javier H. Lohr¹, Ana L. Larralde², Javier Curiale^{3,4}, Rodolfo D. Sánchez^{3,4}, Javier Campo⁵, Gabriel J. Cuello⁶, Denis Sheptyakov⁷, Lukas Keller⁷, Michel Kenzelmann⁷, Gabriela Aurelio⁸**¹Comisión Nacional de Energía Atómica–Laboratorio Argentino de Haces de Neutrones, Centro Atómico Bariloche, Av. Bustillo 9500 R8402AGP, S. C. de Bariloche, Argentina; ²Laboratorio de Cristalografía Aplicada, Escuela de Ciencia y Tecnología, Universidad Nacional de San Martín, Martín de Irigoyen 3100, Campus Miguelete, San Martín (1650), Buenos Aires, Argentina; ³Instituto de Nanociencia y Nanotecnología CNEA-CONICET, Centro Atómico Bariloche, Av. Bustillo 9500 R8402AGP, S. C. de Bariloche, Argentina; ⁴Instituto Balseiro, Universidad Nacional de Cuyo - Comisión Nacional de Energía Atómica, Av. Bustillo 9500 R8402AGP, S. C. de Bariloche, Argentina; ⁵Instituto de Ciencia de Materiales de Aragón (CSIC - Universidad de Zaragoza) and Departamento de Física de Materia Condensada, Universidad de Zaragoza. C/Pedro Cerbuna 12, E-50009 Zaragoza, Spain; ⁶Institut Laue Langevin. 71, Av des Martyrs, BP 156 F-38042 Grenoble, France; ⁷Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland; ⁸Comisión Nacional de Energía Atómica and CONICET Laboratorio Argentino de Haces de Neutrones, Centro Atómico Bariloche, Av. Bustillo 9500 R8402AGP, S. C. de Bariloche, Argentina; javier.lohr@cab.cnea.gov.ar

External Resource:



MS-30-1023-004_b.pdf

4:10pm - 4:30pm

View outside the box: Supramolecular synthon and intermolecular interactions as a directing tool for shaping magnetic behaviour in design of supramolecular architectures of copper(II) complexes**Nikolina Penić, Damir Pajić, Marijana Đaković**FACULTY OF SCIENCE, UNIVERSITY OF ZAGREB, Zagreb, Croatia; peniceva@hotmail.com

External Resource:



MS-30-546-005_b.pdf

4:30pm - 4:50pm

Structural phase transition and magnetic phase diagram of the lacunar spinel GaMo_4Se_8 **Praveen Vir¹, Kieran Routledge², Nicholas Cook², Philip A. E. Murgatroyd², Sheikh J. Ahmed³, Stanislav N. Savvin¹, John B. Claridge³, Jonathan Alaria²**¹Diffraction group, Institut Laue-Langevin (ILL) Grenoble, France; ²Department of Physics, University of Liverpool, United Kingdom;³Department of Chemistry, University of Liverpool, United Kingdom; vir@ill.fr

External Resource:



MS-30-1094-006_b.pdf

4:50pm - 5:10pm

Neutron powder diffraction studies of magnetic transitions in Fe-based orthorhombic perovskites**Juan Pablo Bolletta¹, Antoine Maignan¹, Christine Martin¹, Raúl Ernesto Carbonio²**¹CRISMAT, Normandie Univ, ENSICAEN, UNICAEN, CNRS, Caen, France; ²INFIQC, CONICET-UNC, Córdoba, Argentina; juan-pablo.bolletta@ensicaen.fr

External Resource:





MS-30-792-007_b.pdf

MS-31: Recent advances in instrumentation

Location: **Terrace 2B**

Session Chair: **Ehrenfried Zschech**

Session Chair: **Michele Cianci**

Invited: **Wenbing Yun (USA), Andrew Thomson (France)**

Introduction

2:45pm - 2:50pm

Introduction to session

Ehrenfried Zschech, Michele Cianci



MS-31-1760-001.pdf

2:50pm - 3:20pm

Evolutions in Synchrotron based Integrated Structural Biology at SOLEIL

Andrew Thompson

Synchrotron SOLEIL, St Aubin, France; andrew.thompson@synchrotron-soleil.fr

External Resource: Presentation



MS-31-1380-002_b.pdf

3:20pm - 3:40pm

Optimised high energy data collection in protein crystallography with a CdTe based detector

Selina Lea Sophie Storm^{1,2}, Danny Axford¹, Robin Leslie Owen¹

¹Diamond Light Source, Didcot, United Kingdom; ²EMBL Hamburg, Germany, Germany; selina.storm@embl-hamburg.de

External Resource: Presentation



MS-31-1009-003_b.pdf

3:40pm - 4:00pm

The upgrade of ID29: a novel instrument for Time resolved serial crystallography experiment at the ESRF Extremely Brilliant Source

Daniele de Sanctis

ESRF - The European Synchrotron, Grenoble, France; daniele.de_sanctis@esrf.fr

External Resource: Presentation



MS-31-1069-004_b.pdf

4:00pm - 4:20pm

Development of a high pressure option for neutron scattering experiments at low temperatures and high magnetic fields at the MLZ

Andreas Eich^{1,2}, Karen Friese¹, Micha Hölzle¹, Yixi Su³, Thomas Müller³, Vladimir Hutanu^{2,3}, Muni Kishore Babu Poli^{2,3}, Robert Georgii^{4,5}, Lukas Beddrich^{4,5}, Martin Meven^{2,3}, Andrzej Grzechnik²

¹Jülich Centre for Neutron Science-2/Peter Grünberg-Institute-4, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany; ²Institute for Crystallography, RWTH Aachen University, 52056 Aachen, Germany; ³Jülich Centre for Neutron Science at Heinz Maier-Leibnitz Zentrum, Forschungszentrum Jülich GmbH, 85747 Garching, Germany; ⁴Heinz Maier-Leibnitz Zentrum, Technische Universität München, 85747 Garching, Germany; ⁵Physik-Department E21, Technische Universität München, 85748 Garching, Germany; a.eich@fz-juelich.de

External Resource: Presentation



MS-31-901-005_b.pdf

4:20pm - 4:40pm

MetalJet X-ray Source for time resolved and in-situ SAXS

Julius Hållstedt, Emil Espes, Anasuya Adibhatla

Excillum, Kista, Sweden; julius.hallstedt@gmail.com

External Resource: Presentation



MS-31-964-006_b.pdf

4:40pm - 5:10pm

Holistically Optimized Laboratory XAS Systems

Wenbing Yun, Srivatsan Sechadri, Ian Spink, Ruimin Oiao, Sylvia Lewis
Sigray, Inc., concord, United States of America; wyun@sigray.com

External Resource:



MS-31-1867-007_b.pdf

MS-32: Recent advances in electron crystallography techniques

Location: **Terrace 2A**

Session Chair: **Jim Ciston**

Session Chair: **Mauro Gemmi**

Invited: **Hongyi Xu** (Sweden), **Emanuela Liberti** (UK)

Introduction

2:45pm - 2:50pm

Introduction to session

Jim Ciston, **Mauro Gemmi**



MS-32-1762-001.pdf

2:50pm - 3:20pm

Quantitative electron ptychography for simultaneous light and heavy elements atom counting

Emanuela Liberti^{1,2}, **Arthur N. Moya**¹, **Kevin P. Treder**¹, **Colum M. O'Leary**¹, **Judy S. Kim**^{1,2,3}, **Peter D. Nellist**¹, **Angus I. Kirkland**^{1,2,3}

¹University of Oxford, Oxford, United Kingdom; ²electron Physical Science Imaging Centre (ePSIC), Diamond Light Source, Didcot, UK; ³The Rosalind Franklin Institute, Harwell Campus, Didcot, UK; emanuela.liberti@materials.ox.ac.uk

External Resource:



MS-32-605-002_b.pdf

3:20pm - 3:50pm

Structure Determination of Biomolecules by 3D Electron Diffraction

Hongyi Xu, **Xiaodong Zou**

Department of Materials and Environmental Chemistry, Stockholm University, Stockholm, Sweden; hongyi.xu@mmk.su.se

External Resource:



MS-32-1008-003_b.pdf

3:50pm - 4:10pm

QCBED-DFT: Experimentally constrained density functional theory

Ding Peng¹, **Phillip Nakashima**²

¹Department of Physics, Norwegian University of Science and Technology (NTNU), Trondheim 7491, Norway; ²Department of Materials Science and Engineering, Monash University, Victoria 3800, Australia; ding.peng@ntnu.no

External Resource:



MS-32-840-004_b.pdf

4:10pm - 4:30pm

Precise lattice parameters through distortions refinement using circular harmonics

Petr Brazda, **Lukas Palatinus**

Institute of Physics of the Czech Academy of Sciences, Prague 8, Czech Republic; brazda@fzu.cz

External Resource:



MS-32-788-005_b.pdf

4:30pm - 4:50pm

Direct Imaging of Metal Additives on Au Nanocube Surface Using 4D-STEM

Weilun Li¹, **Bryan D. Esser**¹, **Anchal Yadav**², **Alison M. Funston**^{2,3}, **S. D. Findlay**⁴, **Changlin Zheng**^{5,6}, **Joanne Etheridge**^{1,5}

¹Department of Materials Science and Engineering; ²School of Chemistry; ³ARC Centre of Excellence in Exciton Science; ⁴School of Physics and Astronomy; ⁵Monash Centre for Electron Microscopy, Monash University, Victoria 3800, Australia; ⁶State Key Laboratory of Surface Physics and Department of Department of Physics, Fudan University, Shanghai 200433, China; weilun.li@monash.edu

External Resource:



MS-32-1080-006_b.pdf

4:50pm - 5:10pm

Real space frequency analysis of electron diffuse scattering for lattice distortion determination in real crystals

Jian-Min Zuo, Yu-Tsun Shao, Haw-Wen Hsiao, Renliang Yuan, Qun Yang, Yang Hu

University of Illinois at Urbana-Champaign, Urbana, United States of America; jianzuo@illinois.edu



MS-32-974-007_b.pdf

SMS-2: Exemplary practice in chemical, biological and materials database archiving

Location: 221-2

Session Chair: Suzanna Ward

Session Chair: Genji Kurisu

Invited: Ian Bruno (UK), Stephen Burley (USA)

Introduction

2:45pm - 2:50pm

Introduction to session

Suzanna Ward, Genji Kurisu



SMS-2-1836-001.pdf

2:50pm - 3:20pm

CSD One Million: Reasons why the crystallographic community is exemplary

Ian Bruno, Natalie Johnson, Matthew Lightfoot, Suzanna Ward

The Cambridge Crystallographic Data Centre, Cambridge, United Kingdom; bruno@ccdc.cam.ac.uk

External Resource:



SMS-2-1341-002_b.pdf

3:20pm - 3:50pm

RCSB Protein Data Bank: Celebrating 50 years of the PDB with new tools for understanding and visualizing biological macromolecules in 3D

Stephen K. Burley

Rutgers, The State University of New Jersey, Piscataway, United States of America; sburley@proteomics.rutgers.edu

External Resource:



SMS-2-1629-003_b.pdf

3:50pm - 4:15pm

Behind the scenes - data processing and quality assurance for the ICSD

Annett Steudel, Stephan Rühl

FIZ Karlsruhe - Leibniz-Institut für Informationsinfrastruktur, Eggenstein-Leopoldshafen, Germany; annett.steudel@fiz-karlsruhe.de

External Resource:



SMS-2-1332-004_b.pdf

4:15pm - 4:40pm

The Full Plate: Benefits of simulated and raw data digital patterns in the Powder Diffraction File™

Stacy Gates-Rector, Thomas Blanton, Vesna Bosnic, Soorya Kabekkodu, Justin Blanton

International Centre for Diffraction Data, Newtown Square, United States of America; gates-rector@icdd.com

External Resource:



SMS-2-1314-005_b.pdf

4:40pm - 5:05pm

Protein Data Bank Japan: 20 years and more as the Asian hub for 3D structure and the founding member of the wwPDB

Genji Kurisu

2:45pm - 5:10pm

External Resource:



SMS-2-1637-006_b.pdf

5:10pm - 6:10pm

Afternoon break 2: Poster session A2, exhibition, coffee/tea

Location: **Exhibition and poster area**

Poster - 09 Automation in bio: Automation in biocrystallography

Session Chair: **Santosh Panjikar**

Session Chair: **Melanie Vollmar**



5:10pm - 6:10pm

Poster session abstracts

Radomír Kužel



Poster - 09 Automation in bio-1935-001.pdf

A simple technique to classify diffraction data from dynamic proteins according to individual polymorphs

Thu Nguyen¹, Kim L. Phan², Dima Kozakov¹, Sandra B. Gabelli², Dale F. Kreidler³, Lawrence C. Andrews⁴, Jean Jakoncic³, Rober M. Sweet³, Alexei S. Soares³, Herbert J. Bernstein³

¹Stony Brook University, Stony Brook, NY, 11794-2424, USA; ²Johns Hopkins University, 725 N Wolfe St., Baltimore, MD, 21205, USA;

³Brookhaven National Laboratory, P.O. Box 5000, Upton, NY, 11973-5000, USA; ⁴Ronin Institute for Independent Scholarship, 9515 NE 137th St., Kirkland, WA, 98034, USA

External Resource:



Poster - 09 Automation in bio-1459-002_b.pdf



Poster - 09 Automation in bio-1459-002_c.pdf

Introducing the XtaLAB Synergy Flow

Mark Del Campo¹, Joseph Ferrara¹, Pierre Le Magueres¹, Mathias Meyer², Przemyslaw Stec², Damian Kucharczyk², Mateusz Idzi², Michal Jasnowski², Marcin Grzeszczyk², Artur Wisniewski²

¹Rigaku Americas Corporation, The Woodlands, TX, USA; ²Rigaku Polska Sp. z o.o., Wrocław Poland; mark.delcampo@rigaku.com

External Resource:



Poster - 09 Automation in bio-1355-003_b.pdf

Macromolecular refinement at any resolution using shift field optimization and regularization

Kevin Cowtan, Paul Bond, Scott Hoh

University of York, YORK, United Kingdom



Poster - 09 Automation in bio-1127-004_b.pdf

Faster turnaround of macromolecular crystallography research

Julius Hållstedt

Excillum, Kista, Sweden

External Resource:



Poster - 09 Automation in bio-962-005_b.pdf

Sails: automated model building of carbohydrates

Mihaela Atanasova, Jon Agirre

University of York, York, United Kingdom

External Resource:



Poster - 09 Automation in bio-292-006_b.pdf

Automated crystal shaping to facilitate native SAD phasing

Naohiro Matsugaki, Masahide Hikita, Akira Shinoda, Yusuke Yamada, Toshiya Senda

High Energy Accelerator Research Organization, Tsukuba, Japan

External Resource:





Poster - 09 Automation in bio-1554-007_b.pdf

XALOC, the MX beamline at ALBA synchrotron: Current status and perspectives

Fernando Gil-Ortiz, Xavier Carpena, Barbara M. Calisto, Isidro Crespo, José Maria Álvarez, Jordi S. Andreu, Ricardo Valcarcel, Albert Miret, José Ávila, Jorge Villanueva, Judith Juanhuix, Roeland BOERoer
ALBA SYNCHROTRON, CERDANYOL DEL VALLES, Spain

External Resource:



Poster - 09 Automation in bio-1583-008_b.pdf

Poster - 10: Solution scattering

Session Chair: **Frank Gabel**

Session Chair: **Masaaki Sugiyama**



5:10pm - 6:10pm

Poster session abstracts

Radomír Kužel



Poster - 10-1937-001.pdf

AUC-SAS: Integrated analysis of biomacromolecular structure with analytical ultracentrifugation (AUC) and small-angle scattering (SAS)

Ken Morishima, Rintaro Inoue, Masahiro Shimizu, Aya Okuda, Nobuhiro Sato, Reiko Urade, Masaaki Sugiyama
Kyoto University, Osaka, Japan; morishima@rri.kyoto-u.ac.jp

External Resource:



Poster - 10-1057-002_b.pdf

Establishment of basic techniques related to protein sample preparation for neutron scattering

Aya Okuda, Rintaro Inoue, Ken Morishima, Yasuhiro Yunoki, Masahiro Shimizu, Nobuhiro Sato, Reiko Urade, Masaaki Sugiyama
Kyoto University, Osaka, Japan; okuda.aya.5r@kyoto-u.ac.jp

External Resource:



Poster - 10-1089-003_b.pdf

Subunit dynamics in alpha-crystallin through deuteration-assisted small-angle neutron scattering

Rintaro Inoue¹, Yusuke Sakamaki¹, Takumi Takata¹, Ken Morishima¹, Kathleen Wood², Nobuhiro Sato¹, Aya Okuda¹, Masahiro Shimizu¹, Reiko Urade¹, Noriko Fujii¹, Masaaki Sugiyama¹

¹Kyoto University, Osaka, Japan; ²Australian Nuclear Science and Technology Organization; inoue.rintaro.5w@kyoto-u.ac.jp

External Resource:



Poster - 10-996-004_b.pdf

Dynamics of multi-domain protein ER-60 revealed by small angle X-ray scattering data and molecular dynamics simulations

Masahiro Shimizu, Aya Okuda, Ken Morishima, Nobuhiro Sato, Rintaro Inoue, Reiko Urade, Masaaki Sugiyama
Kyoto University, Osaka, Japan; shimizu.masahiro.3n@kyoto-u.ac.jp

External Resource:



Poster - 10-1389-005_b.pdf

Stoichiometric unfolding of bovine serum albumin by surfactant, as revealed from HPLC/SAXS with online observation of UV-Vis absorption and refractive index.

Yi-Qi Yeh¹, Kuei-Fen Liao¹, Orion Shih¹, Wei-Ru Wu¹, Chun-Jen Su¹, U-Ser Jeng^{1,2}

¹National Synchrotron Radiation Research Center, Hsinchu, Taiwan; ²Department of Chemical Engineering, National Tsing Hua University, Hsinchu 30013, Taiwan

External Resource:





Poster - 10-1273-006_b.pdf

Sterol-crystallin interaction mediated by membranes

Yu-Ting Liu¹, Jui-Kai Chen², Jheng-Hao Lin², Ching-Hsun Yang², Ming-Tao Lee^{1,2}

¹Department of Physics, National Central University, Zhongli, Taiwan; ²National Synchrotron Radiation Research Center, 101 Hsin-Ann Road, Hsinchu Science Park, Hsinchu, Taiwan

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Poster - 10-1253-007_b.pdf

Study of protein-protein interactions of human E3 ubiquitin ligase NEDD4-2 using fluorescence spectroscopy

Rohit Ashok Joshi^{1,2}, Tomas Obsil^{1,2}, Veronika Obsilova¹

¹Department of Structural Biology of Signaling Proteins, Division BIOCEV, Institute of Physiology of the Czech Academy of Sciences, 252 50 Vestec, Czech Republic; ²Department of Physical and Macromolecular Chemistry, Faculty of Science, Charles University, 12843 Prague, Czech Republic.

External Resource:



Poster - 10-1007-008_b.pdf

Determining the role of TIR domain of Interleukin-1 receptor 8 (SIGIRR) in regulating TLR4 signalling

Surekha Nimma¹, Jeffrey Nanson¹, Thomas Ve^{1,2}, Bostjan Kobe^{1,3}

¹University of Queensland, Brisbane, QLD 4072, Australia; ²Institute for Glycomics, Griffith University, Southport, QLD 4222, Australia; ³Institute of Molecular Bioscience, University of Queensland, Brisbane, QLD 4072, Australia

External Resource:



Poster - 10-1254-009_b.pdf

Forbidden reflections induced by unit-cell elastic distortions in paratellurite crystals

A. Petrenko^{1,2}, E. Ovchinnikova^{2,3}, D. Novikov⁴, A. Kulikov^{1,2}, A. Khadiev⁴, N. Marchenkov^{1,2}, M. Zschornak⁵, C. Ludt⁵, K. Kozlovskaya³, V. Dmitrienko¹, A. Blagov^{1,2}

¹FSRC "Crystallography and photonics" RAS, Moscow, Russia; ²NRC "Kurchatov Institute", Moscow, Russia; ³Lomonosov Moscow State University, Moscow, Russia; ⁴DESY, Hamburg, Germany; ⁵Freiburg University of Mining and Technology, Freiberg, Germany; diacon0301@gmail.com

External Resource:



Poster - 10-543-010_b.pdf

A New Biological Small- and Wide-Angle X-ray Scattering Beamline Featured in High Flux, USAXS, and Microbeam at Taiwan Photon Source

KUEIFEN LIAO¹, Yi-Qi Yeh¹, Orion Shih¹, Chun-Jen Su¹, Wei-Ru Wu¹, Chen-An Wang¹, Din-Goa Liu¹, Chien-Hung Chang¹, Liang-Chih Chiang¹, Cheng-Yuan Lin¹, Chia-Feng Chang¹, Cheng-Chih Liang¹, Te-Hui Lee¹, Meng-Chiao Ho², U-Ser Jeng^{1,3}

¹National Synchrotron Radiation Research Center, Hsinchu, Taiwan; ²Institute of biochemical sciences & Institute of biological chemistry, Academia Sinica, Taiwan; ³Department of Chemical Engineering, National Tsing Hua University, Taiwan; liao.kf@nsrc.org.tw

External Resource:



Poster - 10-1255-011_b.pdf

Employing high-end X-ray technologies for laboratory structural biology in Centre of Molecular Structure

Jan Stránský¹, Jiří Pavlíček¹, Andreas Keilbach², Jan Dohnálek¹

¹Institute of Biotechnology, CAS, Vestec u Prahy, Czech Republic; ²Anton Paar GmbH, Anton-Paar-Strasse 20, Graz



Poster - 10-1625-012_b.pdf

Aggregation Forms of Type I Collagen Studied by Simultaneous Small- and Wide-Angle X-ray Scattering

Ying-Jen Shiu¹, Kuei-Fen Liao¹, Je-Wei Chang¹, Orion Shih¹, Chen-An Wang¹, Ting-Wei Hsu¹, Tzu-Jung Lan¹, Yung-Chen Lin¹, Chia-Yu Lin¹, U-Ser Jeng^{1,2}

¹National Synchrotron Radiation Research Center, Hsinchu, Taiwan; ²Department of Chemical Engineering, National Tsing Hua University, Hsinchu, Taiwan; yingjenshiu@gmail.com

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Poster - 10-1870-013_b.pdf

5:10pm - 6:10pm

Poster - 11 Viruses: Structural biology of viruses



Poster session abstracts

Radomir Kužel



Poster - 11 Viruses-1938-001.pdf

Structural Characterization of Endoribonuclease Nsp15 from SARS CoV-2

Youngchang Kim¹, Natalia Maltseva¹, Changsoo Chang¹, Mateusz Wilamowski², Robert Jedrzejczak¹, Jacek Wower³, Glenn Randall², Karolina Michalska¹, Andrzej Joachimiak^{1,2}

¹Argonne National Laboratory, Lemont, United States of America; ²University of Chicago, Chicago, United States of America; ³Auburn University, Auburn, United States of America

External Resource:



Poster - 11 Viruses-1402-002_b.pdf

PDB-KB COVID-19 Data Portal - supporting rapid coronavirus research

Sameer Velankar

EMBL-EBI, Cambridge, United Kingdom

External Resource:



Poster - 11 Viruses-1282-003_b.pdf

3DBionotes Covid-19 Edition

José Ramon Macías¹, Ruben Sanchez-Garcia¹, Pablo Conesa¹, Erney Ramirez-Aportela¹, Marta Martinez Gonzalez¹, Carlos Wert-Carvajal¹, Alberto M. Parra-Perez¹, Joan Segura Mora², Sam Horrell³, Andrea Thorn⁴, Carlos O.S. Sorzano¹, Jose Maria Carazo¹

¹Spanish National Bioinformatics Institute (INB ELIXIR-ES), Biocomputing Unit, National Center for Biotechnology (CNB-CSIC), Instruct Image Processing Center; ²Research Collaboratory for Structural Bioinformatics Protein Data Bank, San Diego Supercomputer Center, University of California, San Diego, La Jolla; ³Diamond Light Source Ltd. (DLS), Oxfordshire, UK; ⁴Institute for Nanostructure and Solid State Physics, HARBOR, Universität Hamburg, Germany

External Resource:



Poster - 11 Viruses-1322-004_b.pdf

Crystal structure of the C24 protein from the Antarctic bacterium *Bizionia argentinensis* JUB59, a putative long tail fiber receptor-binding tip from a novel temperate bacteriophage

Leonardo Pellizza¹, José L. López², Susana Vázquez³, Gabriela Sycz¹, Beatriz G. Guimarães^{4,5}, Jimena Rinaldi¹, Fernando A. Goldbaum¹, Martín Aran¹, Walter P. Mac Cormack^{3,6}, Sebastián Klinke¹

¹Fundación Instituto Leloir, IIBBA-CONICET, Buenos Aires, Argentina; ²Instituto de Bacteriología y Virología Molecular IBAVIM, Universidad de Buenos Aires, Buenos Aires, Argentina; ³Instituto NANOBIOTEC, Universidad de Buenos Aires, Buenos Aires, Argentina; ⁴Synchrotron SOLEIL, Gif-sur-Yvette, France; ⁵Instituto Carlos Chagas - Fund. Oswaldo Cruz, Curitiba, Brazil; ⁶Instituto Antártico Argentino, Buenos Aires, Argentina

External Resource:



Poster - 11 Viruses-608-005_b.pdf

The role of structural biology in pandemic's puzzles: amino acids and short peptides as key players

Joanna Bojarska¹, Vasso Apostolopoulos², John Matsoukas^{3,4}, Jack Feehan^{5,6}, Piotr Zielenkiewicz^{7,8}

¹Technical University of Lodz, Poland; ²Institute for Health and Sport, Victoria University, Melbourne, VIC 3030, Australia; ³NewDrug, Patras Science Park, 26500 Patras, Greece; ⁴Department of Physiology and Pharmacology, Cumming School of Medicine, University of Calgary, Canada; ⁵Institute for Sustainable Industries and Liveable Cities, Victoria University, Melbourne, Australia; ⁶AquaMem Consultants, Rodeo, New Mexico, USA; ⁷Institute of Biochemistry and Biophysics, Polish Academy of Sciences, Pawinskiego 5a, 02-106 Warsaw, Poland; ⁸Department of Systems Biology, Institute of Experimental Plant Biology and Biotechnology, University of Warsaw, Miecznikowa 1, 02-096 Warsaw, Poland; joanna.bojarska@p.lodz.pl

External Resource:





Poster - 11 Viruses-1880-006_b.pdf

Poster - 12 Supramolecular: Theory and practice of supramolecular synthons in crystal engineering



5:10pm - 6:10pm

Session Chair: **Alessia Bacchi**

Session Chair: **Seiji Tsuzuki**

Poster session abstracts

Radomír Kužel



Poster - 12 Supramolecular-1939-001.pdf

Conformational polymorphism of a pharmaceutical cocrystal involving niflumic acid and caffeine

Duane Choquesillo-Lazarte¹, Carolina Alarcón-Payer², Cristóbal Verdugo-Escamilla¹, Milena Di Crisci¹, Jaime Gómez-Morales¹, Alicia Domínguez-Martín³

¹Laboratorio de Estudios Cristalográficos, IACT, CSIC, Armilla (Granada), Spain; ²Hospital Universitario Virgen de las Nieves, Granada, Spain; ³Department of Inorganic Chemistry, University of Granada, Granada, Spain; duane.choquesillo@csic.es

External Resource:



Poster - 12 Supramolecular-1597-002_b.pdf

Crystal structure studies, computational analysis, and hydrogen bonding attributes of halogen bonded sulfonyl Schiff bases

KARTHIK KUMARA^{1,2}, Nani Shankar V. Harohally³, Lokanath N. K.²

¹Department of Physics, School of Sciences-I, JAIN (deemed to be University), Bangalore 560011, India.; ²Department of Studies in Physics, Manasagangotri, University of Mysore, Mysuru 570 006, India.; ³Department of Spice and Flavor Science, CSIR-CFTRI, Mysuru 570020, India.; karthikkumara@jainuniversity.ac.in



Poster - 12 Supramolecular-1624-003_b.pdf

Cocrystals of ethenzamide with polyphenols: Solid state characterization and preliminary evaluation of biopharmaceutical parameters.

Francisco Javier Acebedo-Martínez¹, Carolina Alarcón-Payer², Jaime Gómez-Morales¹, Alicia Domínguez-Martín³, Duane Choquesillo-Lazarte¹

¹Laboratorio de Estudios Cristalográficos, IACT, CSIC, Armilla (Granada), Spain; ²Hospital Universitario Virgen de las Nieves, Granada, Spain; ³Department of Inorganic Chemistry, University of Granada, Granada, Spain; jacebedo@csic.es

External Resource:



Poster - 12 Supramolecular-1599-004_b.pdf

Separation of Lutidine Isomers by Selective Enclathration

Jacky Sorrel Bouanga Boudiombo¹, Hong Su¹, Neil Ravenscroft¹, Susan Bourne¹, Edwin Weber², Luigi Nassimbeni¹

¹University of Cape Town, Cape Town, South Africa; ²Institut für Organische Chemie, TU Bergakademie Freiberg, Leipziger Straße 29, D-09596 Freiberg/Sachs, Germany; bouangabjs@gmail.com

External Resource:



Poster - 12 Supramolecular-313-005_b.pdf



Poster - 12 Supramolecular-313-005_c.pdf

Osme bond: anisotropic distribution of electron density in action

Andrea Pizzi¹, Andrea Daolio¹, Miriam Calabrese¹, Giancarlo Terraneo¹, Antonio Frontera², Giuseppe Resnati¹

¹Politecnico di Milano, Milano, Italy; ²Universitat de les Illes Balears; andrea.pizzi@polimi.it

External Resource:



Poster - 12 Supramolecular-1684-006_b.pdf



Poster - 12 Supramolecular-1684-006_c.pdf

Organic homomolecular crystals with the shortest period of about 4 Å: the role of halogen atoms according to the CSD statistics

Olga V. Grineva

Chemistry Department of Moscow M. V. Lomonosov State University, Moscow, Russia; ovg@phys.chem.msu.ru

External Resource:



Poster - 12 Supramolecular-1714-007_b.pdf

Electrostatic self-assembly of organic crystals from charged macrocycles

Kateryna Kravets, Mykola Kravets, Volodymyr Sashuk, Oksana Danylyuk

Institute of Physical Chemistry Polish Academy of Sciences, Warsaw, Poland; kkravets@ichf.edu.pl

External Resource:



Poster - 12 Supramolecular-1691-008_b.pdf

Crystal engineering concepts in the design and synthesis of a series of novel, structurally related spin-crossover materials, characterized by variable temperature single crystal X-ray diffraction.

Lee Terence Birchall, Helena Shepherd

School of Physical Sciences, Ingram Building, University of Kent, Canterbury, CT2 7NH; ltb7@kent.ac.uk

External Resource:



Poster - 12 Supramolecular-1042-009_b.pdf

Synthesis, Crystal Structure, Vibrational Study and DFT Computation of Barium Dihydrogenomonophosphate $\text{Ba}(\text{H}_2\text{PO}_4)_2$

Rachida Oubouaza¹, Mark Benson², Jakub Wojciechowski³, Samir Chtita⁴, Malika Tridane⁵, Said Belaouad⁶

¹Laboratory of chemistry-physics of materials LCPM, Faculty of Sciences Ben M'Sik, B.P7955, Hassan II University of Casablanca, Morocco;; ²Institute of General and Ecological Chemistry, Łódź University of Technology, 116 Zeromskiego St., 90-924 Lodz, Poland; ³Department of Chemistry, University of Liverpool, CrownStreet, Liverpool L697ZD, UK;; ⁴Laboratory of chemistry-physics of materials LCPM, Faculty of Sciences Ben M'Sik, B.P7955, Hassan II University of Casablanca, Morocco;; ⁵Regional Center of the education and training trades Anfa Bd BirAnzarane Casablanca. Morocco;; ⁶Laboratory of chemistry-physics of materials LCPM, Faculty of Sciences Ben M'Sik, B.P7955, Hassan II University of Casablanca, Morocco;; oubouazarachida01@gmail.com

External Resource:



Poster - 12 Supramolecular-882-010_b.pdf

Tetrel bond: dipyriddy methylene as a donor site

Andrea Daolio, Andrea Pizzi, Giuseppe Resnati, **Miriam Calabrese**

Politecnico di Milano, Torino, Italy; miriam.calabrese@polimi.it

External Resource:



Poster - 12 Supramolecular-669-011_b.pdf



Poster - 12 Supramolecular-669-011_c.pdf

The N-methylammonium moiety: A tetrel bond donor site

Andrea Daolio¹, Giancarlo Terraneo¹, Alessandro Genoni², Giuseppe Resnati¹

¹Politecnico di Milano, Milano, Italy; ²Université de Lorraine, Vandoeuvre-lès-Nancy, France; andrea.daolio@polimi.it

External Resource:



Poster - 12 Supramolecular-418-012_b.pdf

Poster - 13 Data: Crystallographic data

Session Chair: **Olivier C. Gagné**

Session Chair: **Anton Oliynyk**



5:10pm - 6:10pm

Poster session abstracts

Radomir Kužel



Poster - 13 Data-1940-001.pdf

X-ray structural analysis of crystalline materials at the XSA/Belok beamline at synchrotron radiation source of the Kurchatov institute

Vladimir Lazarenko¹, Yan Zubavichus², Pavel Dorovatovskii¹, Roman Svetogorov¹

¹NRC "Kurchatov institute", Moscow, Russian Federation; ²Borisev Institute of Catalysis SB RAS, Novosibirsk, Russian Federation; vladimir.a.lazarenko@gmail.com

External Resource:  Presentation



Poster - 13 Data-338-002_b.pdf

Using the Gold Standard for data archival at kilohertz speeds

Aaron Brewster¹, Herbert Bernstein², Andreas Förster³, Graeme Winter⁴

¹Lawrence Berkeley National Lab, Albany, United States of America; ²Ronin Institute for Independent Scholarship; ³DECTRIS Ltd;

⁴Diamond Light Source Ltd; asbrewster@lbl.gov

External Resource:  Presentation



Poster - 13 Data-1339-003_b.pdf

DC⁷, A very efficient lattice comparison metric

Herbert J. Bernstein¹, Lawrence C. Andrews²

¹Ronin Institute for Independent Scholarship, c/o NSLS II, Brookhaven National Laboratory, Upton, NY 11973-5000, USA; ²Ronin Institute for Independent Scholarship, 9515 NE 137th St, Kirkland, WA, 98034-1820, USA; yayahjb@gmail.com

External Resource:  Presentation



Poster - 13 Data-1230-004_b.pdf



Poster - 13 Data-1230-004_c.pdf

Seed-skewness algorithm for x-ray diffraction signal detection in the time-resolved synchrotron Laue photocrystallography

Dariusz Krzysztof Szarejko, Radosław Kamiński, Piotr Łaski, Katarzyna N. Jarzemska

Department of Chemistry, Warsaw University, Warszawa, Poland; kontakt@szarejko.dariusz.pl

External Resource:  Presentation



Poster - 13 Data-732-005_b.pdf

Metadata for better data - Growing and improving the Cambridge Structural Database

Natalie Johnson, Seth B Wiggan, Suzanna C Ward, Ian Bruno

Cambridge Crystallographic Data Centre, Cambridge, United Kingdom; njohnson@ccdc.cam.ac.uk

External Resource:  Presentation



Poster - 13 Data-1611-006_b.pdf

Chemical annotation in the Crystallography Open Database

Andrius Merkys¹, Antanas Vaitkus¹, Algirdas Grybauskas¹, Aleksandras Kononov¹, Miguel Quirós Olozábal², Saulius Gražulis¹

¹Vilnius University Life Sciences Center, Saulėtekio al. 7, 10257 Vilnius, Lithuania; ²Departamento de Química Inorgánica, Universidad de Granada, 18071, Granada, Spain; andrius.merkys@gmc.vu.lt

External Resource:  Presentation



Poster - 13 Data-1476-007_b.pdf

Role of hydrogen bonding in modifications of impact sensitivities of high energetic materials: evidence from crystal structures and quantum chemical calculations

Dušan Ž. Veljković¹, Danijela S. Kretić¹, Ivana S. Veljković², Dušan P. Malenović¹, Dragan B. Ninković³, Snežana D. Zarić¹

¹University of Belgrade - Faculty of Chemistry, Studentski trg 12 - 16, Belgrade, Serbia; ²University of Belgrade - Institute of Chemistry, Technology and Metallurgy - National Institute of the Republic of Serbia, Njegoševa 12, Belgrade, Serbia; ³Innovation center of the Faculty of Chemistry, Studentski trg 12-16, Belgrade, Serbia; vdusan@chem.bg.ac.rs

External Resource:  Presentation



Poster - 13 Data-1512-008_b.pdf

Improvements to the data search and validation functionality in the Crystallography Open Database

Antanas Vaitkus¹, Andrius Merkys¹, Algirdas Grybauskas¹, Aleksandras Kononovos¹, Miguel Quirós Olozábal², Saulius Gražulis^{1,3}

¹Vilnius University, Life Sciences Center, Institute of Biotechnology, Saulėtekio 7, LT-10257 Vilnius, Lithuania; ²Departamento de Química Inorgánica, Universidad de Granada, 18071, Granada, Spain; ³Vilnius University, Faculty of Mathematics and Informatics, Naugarduko 24, LT-03225 Vilnius, Lithuania; antanas.vaitkus@bti.vu.lt



Poster - 13 Data-1551-009_b.pdf

A “post-mortem” analysis of radiation damage in the Protein Data Bank with the B_{net} metric

Kathryn Shelley^{1,2}, Elspeth Garman²

¹School of Chemistry, University of Bristol, Cantock's Close, Bristol, BS8 1TS, United Kingdom; ²Dept of Biochemistry, University of Oxford, Oxford, OX1 3QU, United Kingdom

External Resource: Presentation



Poster - 13 Data-1708-010_b.pdf

Data treatment and data storage at the BioSAXS beamline TPS 13A

Orion Shih¹, Chun-Jen Su¹, Yi-Qi Yeh¹, Kuei-Fen Liao¹, Je-Wei Chang¹, Chen-An Wang¹, Wei-Ru Wu¹, U-Ser Jeng^{1,2}

¹National Synchrotron Radiation Research Center, Hsinchu Science Park, Hsinchu 30076, Taiwan; ²Department of Chemical Engineering, National Tsing Hua University, Hsinchu 30013, Taiwan; shih.orion@nsrrc.org.tw

External Resource: Presentation



Poster - 13 Data-1209-011_b.pdf

Poster - 14 Instrumentation: Advances in instrumentation

Session Chair: **Michele Cianci**

Session Chair: **Ehrenfried Zschech**



5:10pm - 6:10pm

Poster session abstracts

Radomír Kužel



Poster - 14 Instrumentation-1941-001.pdf

MicroMAX – new opportunities in macromolecular crystallography

Thomas Ursby, Oskar Aurelius, Monika Bjelčić, Aleksander Cehovin, Ana Gonzalez, Ishkhan Gorgisyan, Mirko Milas, Jie Nan, Peter Sondhauss, Meghdad Yazdi

MAX IV Laboratory, Lund University, Lund, Sweden; thomas.ursby@maxiv.lu.se

External Resource: Presentation



Poster - 14 Instrumentation-1150-002_b.pdf

Serial and Macromolecular Crystallography at beamline P11, Petra III

Johanna Hakanpää¹, Sofiane Saouane¹, Guillaume Pompidor¹, Eva Crosas¹, Jan Meyer¹, Bernhard Kistner¹, Alessandra Henkel², Spyros Chatziefthymiou¹, Thomas A. White³, Dominik Oberthür³

¹Photon Science, Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany; ²University of Lübeck, Lübeck, Germany; ³Center for Free-Electron Laser Science, Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany; johanna.hakanpaa@desy.de



Poster - 14 Instrumentation-1099-003_b.pdf

Non-attended data acquisition in the protein lab using the SCOUT sample changer

Michael Mrosek

Bruker AXS GmbH, Karlsruhe, Germany; michael.mrosek@bruker.com

External Resource: Presentation



Poster - 14 Instrumentation-984-004_b.pdf

Beamline setup & calibration quality control for synchrotron MX beamlines

David Aragao, Nathan Cowieson

Diamond Light Source, Harwell Science and Innovation Campus, Chilton, Didcot, OX11 0DE, UK; david.aragao@diamond.ac.uk

External Resource: Presentation



Poster - 14 Instrumentation-1212-005_b.pdf

DanMAX – The new materials science beamline at MAX IV

Mads Ry Vogel Jørgensen^{1,3}, **Daniel Risskov Sørensen**^{1,3}, **Innokenty Kantor**^{2,3}, **Silvia Forcat Oller**³

¹Department of Chemistry & iNANO, Aarhus University, Denmark; ²Department of Physics, Technical University of Denmark, Denmark;

³MAX IV Laboratory, Lund University, Sweden; mads@chem.au.dk

External Resource:



Poster - 14 Instrumentation-571-006_b.pdf

Pushing the Limits of Microfocus X-Ray Sealed Tube Sources for Crystallography

Juergen Graf¹, **Tobias Stuerzer**², **Matthew Benning**³, **Roger Durst**², **Paul Radcliffe**¹, **Carsten Michaelson**¹

¹Incoatec GmbH, Geesthacht, Germany; ²Bruker AXS GmbH, Karlsruhe, Germany; ³Bruker AXS LLC, Madison WI, USA;

graf@incoatec.de

External Resource:



Poster - 14 Instrumentation-1017-007_b.pdf

Development of high-speed capillary spinner cell for *in-situ* powder diffraction under gas pressure control

Shogo Kawaguchi¹, **Michitaka Takemoto**¹, **Kunihisa Sugimoto**^{1,2}, **Hiroataka Ashitani**³, **Yoshiki Kubota**³

¹Japan Synchrotron Radiation Research Institute (JASRI), SPring-8, Sayo, Hyogo, 679-5198, Japan; ²Institute for Integrated Cell-Material Sciences, Kyoto University, Kyoto 606-8501, Japan.; ³Department of Physical Science, Osaka Prefecture University, Sakai, Osaka 599 8531, Japan; kawaguchi@spring8.or.jp

External Resource:



Poster - 14 Instrumentation-1517-008_b.pdf

Applications of X-ray diffraction for microcrystalline sample using the latest single crystal laboratory systems.

Hiroyasu Sato, **Takashi Matsumoto**, **Takashi Kikuchi**, **Akihito Yamano**

Rigaku Corporation, Tokyo, Japan; h-sato@rigaku.co.jp

External Resource:



Poster - 14 Instrumentation-1521-009_b.pdf

Home-made capillary mounting setup for shaky hands

Bertrand Georges Marcel Fournier

Institut Gallien Paris-Saclay, CNRS UMR 8612, Université Paris-Saclay, 92296 Châtenay-Malabry, France.; bertrand.fournier@u-psud.fr

External Resource:



Poster - 14 Instrumentation-1549-010_b.pdf

Handling of radioactive materials prior to analysis by X-ray powder diffraction

Claudia Aparicio, **Rosnecký Vit**

Centrum výzkumu Řež s.r.o. (Research Centre Řež), Husinec-Řež, Czech Republic; claudia.aparicio@cvrez.cz

External Resource:



Poster - 14 Instrumentation-1333-011_b.pdf



Poster - 14 Instrumentation-1333-011_c.pdf

The latest X-ray analysis solutions from Anton Paar

Andrew O. F. Jones, **Marius Kremer**, **Timo Müller**, **Barbara Pühr**, **Benedikt Schrode**

Anton Paar GmbH, Graz, Austria; andrew.jones@anton-paar.com

External Resource:





Poster - 14 Instrumentation-1398-012_b.pdf

Non-ambient X-ray diffraction – a further dimension in crystallography

Barbara Puhr, Andrew O.F. Jones, Marius Kremer, Timo Müller, Benedikt Schrode
Anton Paar GmbH, Graz, Austria; barbara.puhr@anton-paar.com

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Poster - 14 Instrumentation-1431-013_b.pdf

X-ray Corelab @HZB: A user lab for multi-purpose materials research

Michael Tovar¹, René Gunder¹, Susan Schorr^{1,2}

¹Helmholtz-Zentrum Berlin, Germany; ²Freie Universität Berlin, Germany; tovar@helmholtz-berlin.de

External Resource:



Poster - 14 Instrumentation-1608-014_b.pdf

MGML - Materials Growth & Measurement Laboratory

Pavel Javorský¹, Jan Prokleška¹, Klára Uhlířová¹, Petr Čermák¹, Milan Dopita¹, Martin Žáček²

¹Charles University, Prague, Czech Republic; ²Institute of Physics, CAS, Prague, Czech Republic; javor@mag.mff.cuni.cz

External Resource:



Poster - 14 Instrumentation-1695-015_b.pdf

Core Facility for Crystallographic and Biophysical Research to support the development of medicinal products

Jan Kutner, Maria Górna, Maura Malińska, Monika Wanat, Daria Dawidziak, Katarzyna Polak, Mikołaj Kuska, Weronika Lidwin, Marlena Kisiała, Szymon Sutula, Krzysztof Woźniak

University of Warsaw, Biological and Chemical Research Centre, Core Facility for Crystallography and Biophysics, 101 Zwirki i Wigury, 02-089 Warsaw, Poland; jkutner@chem.uw.edu.pl

External Resource:



Poster - 14 Instrumentation-1726-016_b.pdf

Rigaku's SmartLab XRD tool: All cutting-edge technologies in one instrument.

Artem Shalimov

Rigaku Europe SE, Neu-Isenburg, Germany; artem.shalimov@rigaku.com

External Resource:



Poster - 14 Instrumentation-1716-017_b.pdf

Poster - 15 Films: Crystallographic analysis of thin films and surfaces

Session Chair: **Milan Dopita**



5:10pm - 6:10pm

Poster session abstracts

Radomír Kužel



Poster - 15 Films-1942-001.pdf

Investigating the crystallization behavior of Ge-rich GST PCMs with in-situ synchrotron XRD

Philipp Hans¹, Christophe Guichet¹, Cristian Mocuta², Marie Ingrid Richard^{1,3}, Daniel Benoit⁴, Philippe Boivin⁵, Yannick Le-Frèc⁴, Roberto Simola⁵, Olivier Thomas¹

¹Aix-Marseille Université, CNRS, IM2NP UMR 7334, Marseille, France; ²Synchrotron SOLEIL, Saint-Aubin, France; ³ID01/ESRF, The European Synchrotron, 71 rue des Martyrs, 38043 Grenoble, France; ⁴STMicronics, 850 rue Jean Monnet, 38920 Crolles, France; ⁵STMicronics, 190 Ave Coq, 13106 Rousset, France; philipp.hans@univ-amu.fr

External Resource:





Poster - 15 Films-1046-002_b.pdf

Self-consistent diffraction stress analysis for estimating stress and composition of alloy films

Takashi Harumoto, Ji Shi, Yoshio Nakamura

Tokyo Institute of Technology, Tokyo, Japan; harumoto.t.aa@m.titech.ac.jp

External Resource:



Poster - 15 Films-1206-003_b.pdf

Twin domains of ScN (001) films on MgO (001)

Esther de Prado, Joris More-Chevalier, Stanislav Cichoň, Ján Lančok

Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic; prado@fzu.cz

External Resource:



Poster - 15 Films-1621-004_b.pdf

Phase formations in tungsten carbide films deposited by reactive magnetron sputtering

Lea Haus^{1,2}, Martin Thümmel¹, Julia Wöckel², Christina Wüstefeld¹, Matthias Müller², David Rafaja¹

¹Institute of Materials Science, TU Bergakademie Freiberg, Freiberg, Germany; ²Plasma Technology, Robert Bosch Manufacturing Solutions GmbH, 70442 Stuttgart, Germany; Lea.Haus@de.bosch.com

External Resource:



Poster - 15 Films-1491-005_b.pdf

Laboratory and synchrotron rocking curve imaging for crystal lattice misorientation mapping

Petr Mikulík, Ondřej Caha, Mojmir Meduňa

Masaryk University, Brno, Czech Republic; mikulik@physics.muni.cz

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Poster - 15 Films-1713-006_b.pdf

Titanium surface modified by nitrogen ion implantation

Jan Drahokoupil¹, Petr Vičák², Miroslav Lebeda^{1,2}

¹Institute of Physics, AS CR, Na Slovance 2, 182 21 Prague, Czech Republic; ²Faculty of Mechanical Engineering, Czech Technical University in Prague, Technická 4, 16607 Prague, Czech Republic; draho@fzu.cz

External Resource:



Poster - 15 Films-1616-007_b.pdf

Ion implantation into ZrNb nanometric multilayers

Miroslav Karlík^{1,2}, Nabil Daghbouj³, Jan Lorinčík⁴, Tomáš Polcar³, Mauro Callisti⁵, Vladimír Havránek⁶

¹Charles University, Faculty of Mathematics and Physics, Praha 2, Czech Republic; ²Czech Technical University in Prague, Department of Materials, Praha 2, Czech Republic; ³Czech Technical University in Prague, Department of Control Engineering, Praha 6, Czech Republic; ⁴Research Centre Řež, Husinec-Řež, Czech Republic; ⁵Department of Materials Science and Metallurgy, University of Cambridge, UK; ⁶Nuclear Physics Institute CAS, 250 68 Řež, Czech Republic; Miroslav.Karlik@fffi.cvut.cz

External Resource:



Poster - 15 Films-1848-008_b.pdf

Poster - 16 Texture, defects: Texture, strain, stress, real structure

Session Chair: **David Rafaja**



5:10pm - 6:10pm

Poster session abstracts

Radomír Kužel



Poster - 16 Texture, defects-1943-001.pdf

X-ray peak profile analysis with variance method for the evaluation of dislocation microstructure of copper single crystals loaded in the gigacycle fatigue domain

Doriana Vinci¹, Olivier Castelnau¹, Vincent Jacquemain¹, Christophe Cheuleu¹, Vincent Michel¹, Véronique Favier¹, Cristian Macuta², Nicolas Ranc¹

¹Laboratoire PIMM, Arts et Métiers Institute of Technology, CNRS, HESAM Université, Paris, France; ²Synchrotron SOLEIL, France; doriana.vinci@ensam.eu

External Resource:



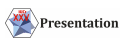
Poster - 16 Texture, defects-1214-002_b.pdf

Shape and lattice deformation contributions to powder scattering

Alberto Leonardi^{1,2}, Matteo Leoni³

¹ISIS Neutron and Muon Facility, UKRI-Science and Technical Facility Council, Didcot, United Kingdom; ²Institute for Multiscale Simulation, Friedrich-Alexander University Erlangen-Nürnberg; ³Saudi Aramco Research & Development Center; alberto.leonardi@stfc.ac.uk

External Resource:



Poster - 16 Texture, defects-1152-003_b.pdf

Getting the most out of neutron powder diffraction - Revealing the microstructure evolution during sintering of magnetic nano-particles using parametric refinement

Frederik H Gjorup, Mathias Mørch, Jakob Ahlburg, Jennifer Hölscher

Aarhus University, Department of Chemistry and Interdisciplinary Nanoscience Center (iNANO), Aarhus C, Denmark; fgjorup@chem.au.dk

External Resource:



Poster - 16 Texture, defects-1199-004_b.pdf

Texture analysis of strongly oriented MAPbI₃ layers using fast reciprocal-space mapping

Lukáš Horák¹, Amalraj Peter Amalathas², Jakub Holovsky^{2,3}

¹Charles University, Faculty of Mathematics and Physics, Prague, Czech Republic; ²Centre for Advanced Photovoltaics, Faculty of Electrical Engineering, Czech Technical University in Prague, 166 27 Prague, Czech Republic; ³Institute of Physics, Czech Academy of Sciences, 162 00 Prague, Czech Republic; horak@karlov.mff.cuni.cz

External Resource:



Poster - 16 Texture, defects-1538-005_b.pdf

Understanding the Residual Strain Distribution as a Function of Depth in Alumina/ Stainless Steel Brazing Joint

Chun Li

Harbin Institute of Technology, Harbin, China, People's Republic of; chun.li@hit.edu.cn

External Resource:



Poster - 16 Texture, defects-1655-006_b.pdf

Induced ferroelectric phase transformation in polycrystalline BaTiO₃

Lucas Lemos da Silva, Manuel Hinterstein

Karlsruhe Institute of Technology, Karlsruhe, Germany; lucas.silva@kit.edu

External Resource:



Poster - 16 Texture, defects-1693-007_b.pdf

High-resolution neutron three axis diffractometer for studies of elastic and plastic deformation of polycrystalline materials

Pavol Mikula, Vasyi Ryukhtin, Jan Šaroun, Pavel Strunz

Nuclear Physics Institute ASCR, v.v.i., Řež, Czech Republic; mikula@ujf.cas.cz

External Resource:



Poster - 16 Texture, defects-997-008_b.pdf

Microstrain and texture in rotary swaged W-Ni-Co pseudoalloy

Pavel Strunz¹, Radim Kocich², Přemysl Beran^{1,3}, Lenka Kunčíková², David Canelo-Yubero¹, Charles Hervoches¹

¹Nuclear Physics Institute, Řež, Czech Republic; ²Faculty of Materials Science and Technology, VŠB-Technical University of Ostrava, 70800 Ostrava-Poruba, Czech Republic; ³European Spallation Source ERIC, 225 92 Lund, Sweden; strunz@ujf.cas.cz

External Resource:



Poster - 16 Texture, defects-1859-009_b.pdf

Deformation behavior of extruded ZN11 magnesium plate

Daria Drozdenko¹, Klaudia Fekete¹, Jan Bohlen², Sangbong Yi², Patrik Dobroň¹

¹Charles University, Faculty of Mathematics and Physics, Department of Physics of Materials, Prague, Czech Republic; ²Helmholtz-Zentrum Hereon, Institute of Material and Process Design, Department of Material Design, Geesthacht, Germany; drozdenko@karlov.mff.cuni.cz

External Resource:



Poster - 16 Texture, defects-1856-010_b.pdf



Poster - 16 Texture, defects-1856-010_c.pdf

KN-10: Gjonnes medal lecture

Location: **Terrace 2A**

Session Chair: **Louisa Meshi**

Ute Kolb, Sven Hovmöller

Gjonnes medal

The development of automated diffraction tomography

Ute Kolb

Johannes Gutenberg-University Mainz, Mainz, Germany; kolb@uni-mainz.de

External Resource:



KN-10-1851-001_b.pdf

Electron crystallography - from slow 2D of simple structures to rapid crystal structure determinations in 3D of very complex structures

Sven Hovmöller

Stockholm university, Stockholm, Sweden; sven.hovmoller@mmk.su.se

External Resource:



KN-10-1852-002_b.pdf

KN-11: Dithiadiazolyl radicals as building blocks for molecular magnetic materials

Location: **Terrace 2B**

Session Chair: **Václav Petříček**

Delia Haynes

Dithiadiazolyl radicals as building blocks for molecular materials

Delia A. Haynes

Stellenbosch University, Stellenbosch, South Africa; dhaynes@sun.ac.za

External Resource:



KN-11-1377-001_b.pdf

KN-12: Structural hybrid methods to probe membrane transport nanomachines in pathogenic bacteria

Location: **Club A**

Session Chair: **Julie Bouckaert**

Natalie Strynadka

Hybrid structural methods to probe atomic features of the Type III Secretion Injectisome of Pathogenic Bacteria

Natalie Strynadka

UBC, Vancouver, Canada; ncjs@mail.ubc.ca

External Resource:



KN-12-1660-001_b.pdf

7:15pm - 10:15pm

IUCr-2: IUCr assembly
Location: **Club H**
Session Chair: **Sven Lidin**
Session Chair: **Luc Van Meervelt**
Session Chair: **Alex Ashcroft**
IUCr assembly 2
Videos: Outreach and education - IUCr journals - Calgary bid - Berlin bid

Date: Tuesday, 17/Aug/2021

9:00am - 9:50am

KN-13: Structural flexibility and disorder in functional materials
Location: **Terrace 2A**
Session Chair: **Brendan Kennedy**
Andrew Goodwin

Structural flexibility and disorder in functional materials

Andrew Goodwin

University of Oxford, Oxford, United Kingdom; andrew.goodwin@chem.ox.ac.uk

External Resource:



KN-13-1464-001_b.pdf

9:00am - 9:50am

KN-14: Quantum crystallography and spintronic materials
Location: **Terrace 2B**
Session Chair: **Krzysztof Wozniak**
Piero Macchi

Quantum crystallography and spintronic materials

PIERO MACCHI

POLITECNICO DI MILANO, MILANO, Italy; piero.macchi@polimi.it

External Resource:



KN-14-970-001_b.pdf

9:00am - 9:50am

KN-15: Time resolved macromolecular crystallography
Location: **Club A**
Session Chair: **Ivana Kuta Smatanova**
Arwen R Pearson

9:00am - 10:00am
Time-resolved macromolecular crystallography: no longer a niche pursuit?

Arwen R Pearson

University of Hamburg, Hamburg, Germany; arwen.pearson@cfel.de

External Resource:



KN-15-1659-001_b.pdf

9:50am - 10:20am

Morning break 3: Exhibition, posters, coffee/tea
Location: **Exhibition and poster area**

MS-33: CryoEM for macromolecules - from single particles to microcrystals
Location: **Club A**
Session Chair: **Jan Pieter Abrahams**
Session Chair: **Jiri Novacek**
Invited: **Nenad Ban** (Switzerland), **Dimple Karia** (Netherlands)

Introduction
10:20am - 10:25am
Introduction to session
Jan Pieter Abrahams, Jiří Nováček



MS-33-1763-001.pdf

10:25am - 10:55am

Structural basis of SARS-CoV-2 translational shutdown and programmed ribosomal frameshifting

Nenad Ban

ETH Zurich, Zurich, Switzerland

External Resource:



MS-33-1418-002_b.pdf

10:55am - 11:25am

Home source for cryo-EM

Dimple Karia¹, Adrian Koh¹, Zuzana Hlavenkova², Milos Malinsky², Vojtech Dolezal², Alevtyna Yakushevskaya¹, Lingbo Yu¹, Abhay Kotecha¹

¹Thermo Fisher Scientific, Materials and Structural Analysis Division, Achtseweg Noord, Eindhoven, Netherlands; ²Thermo Fisher Scientific Brno s.r.o, Materials & Structural Analysis, Brno, Czech Republic

External Resource:



MS-33-906-003_b.pdf

11:25am - 11:50am

High-resolution structures of immature and chimeric flaviviruses reveal key features redefining viral architecture and maturation

Joshua Hardy¹, Natalee Newton², Naphak Modhiran², Connor Scott², Hari Venugopal¹, Laura Vet², Paul Young², Roy Hall², Jody Hobson-Peters², Daniel Watterson², Fasseli Coulibaly¹

¹Monash University, Clayton, VIC, Australia; ²The University of Queensland, Brisbane, QLD, Australia

External Resource:



MS-33-806-004_b.pdf

11:50am - 12:15pm

Receptor induced rearrangements of capsid and genome prime rhinovirus 14 for activation and uncoating

Dominik Hrebik, Tibor Füzik, Mária Gondová, Lenka Šmerdová, Athanassios Adamopoulos, Ondrej Šedo, Zbyněk Zdráhal, Pavel Plevka

CEITEC MU, Brno, Czech Republic

External Resource:



MS-33-1190-005_b.pdf

12:15pm - 12:40pm

M. tuberculosis enolase: Crystal and Cryo-EM structures provide insights into 2-phosphoglycerate binding and catalysis

Mohammed Ahmad¹, Bhavya Jha¹, Sucharita Bose², Satish Tiwari¹, Abhisek Dwivedy¹, Richard Mariadasse³, Ravikant Pal¹, Tanya Parish⁴, J Jayekanthan³, Vinothkumar kutti Ragunath², Bichitra Kumar Biswal¹

¹National Institute of Immunology, New Delhi, India; ²National Centre for Biological Sciences, Bangalore 560065, India; ³Alagappa University, Karaikudi, Tamil Nadu 630003, India; ⁴Infectious Disease Research Institute, 1616 Eastlake Avenue E, Suite 400, Seattle, WA 98102, United States; ahmad@nii.ac.in



MS-33-474-006_b.pdf

MS-34a: Structural biology of enzymes, mechanism and regulation

Location: Club B

Session Chair: Mirjam Czjzek

Invited: Liang Wu (UK), Orsolya Barabas (Germany)

Introduction

10:20am - 10:25am

Introduction to session

Mirham Czjzek



MS-34a-1764-001.pdf

10:25am - 10:55am

Adventures in heparan sulfate degradation

Liang Wu¹, Zachary Armstrong², Casper de Boer³, Vincent Lit³, Gijs Ruijgrok³, Uri Barash⁴, Ilanit Boyango⁴, Neta Ilan⁴, Israel Vlodavsky⁴, Hermen S Overkleef³, Gideon J Davies²

¹The Rosalind Franklin Institute, Didcot, OX11 0FA, United Kingdom; ²Department of Chemistry, University of York, York, YO10 5DD, United Kingdom; ³Department of Bio-organic Synthesis, Leiden Institute of Chemistry, Leiden University, Einsteinweg 55, 2333 CC Leiden, The Netherlands; ⁴Technion Integrated Cancer Center (TICC), The Bruce Rappaport Faculty of Medicine, Technion, Haifa 31096, Israel

External Resource:





MS-34a-995-002_b.pdf

10:55am - 11:25am

High-resolution structure and reaction cycle of Fatty Acid Photodecarboxylase: anatomy of a crime scene

Damien Sorigue¹, Kyprianos Hadjidemetriou², Stéphanie Blangy¹, Guillaume Gotthard³, Pierre Legrand⁴, Didier Nurizzo³, Antoine Royant⁵, Catherine Berthomieu¹, Martin Weik², Tatiana Domratheva⁵, Klaus Brettel⁶, Martin Vos⁷, Ilme Schlichting⁸, Pavel Muller⁶, Fred Beisson¹, **Pascal Arnoux¹**

¹CEA, Saint Paul lez Durance, France; ²IBS, Grenoble, France; ³ESRF, Grenoble, France; ⁴SOLEIL, Gif-sur-Yvette, France;

⁵Lomonosov Moscow State University, Moscow, Russia; ⁶12BC, Gif-sur-Yvette, France; ⁷Ecole Polytechnique, Palaiseau, France; ⁸MPI, Heidelberg, Germany

External Resource:



MS-34a-787-003_b.pdf

11:25am - 11:45am

Structural insights into the enzymatic mechanism of lytic polysaccharide monooxygenases

Flora Meilleur

NC State / ORNL, Raleigh, United States of America

External Resource:



MS-34a-141-004_b.pdf

11:45am - 12:05pm

Structural studies on a unique glucosamine kinase unveil a novel enzyme family

Jose Antonio Manso^{1,2}, Daniela Nunes Costa^{3,4}, Sandra Macedo Ribeiro^{1,2}, Nuno Empadinhas^{3,4}, Pedro Jose Barbosa Pereira^{1,2}

¹IBMC-Instituto de Biologia Molecular e Celular, Universidade do Porto, Porto, Portugal; ²Instituto de Investigação e Inovação em Saúde, Universidade do Porto, Porto, Portugal; ³CNC-Center for Neuroscience and Cell Biology, University of Coimbra, Coimbra, Portugal; ⁴PhD Program in Experimental Biology and Biomedicine (PDBEB), University of Coimbra, Coimbra, Portugal

External Resource:



MS-34a-1240-005_b.pdf

12:05pm - 12:25pm

Biosynthesis of mycobacterial methylmannose polysaccharides requires a unique 1-O-methyltransferase specific for 3-O-methylated mannosides

Jorge Ripoll-Rozada^{1,2}, Mafalda Costa³, José Antonio Manso^{1,2}, Ana Maranhã³, Vanessa Miranda⁴, André Sequeira⁴, Maria Rita Ventura⁴, Sandra Macedo-Ribeiro^{1,2}, Nuno Empadinhas^{3,5}, Pedro José Barbosa Pereira^{1,2}

¹IBMC – Instituto de Biologia Molecular e Celular, Universidade do Porto, 4200-135 Porto, Portugal.; ²Instituto de Investigação e Inovação em Saúde, Universidade do Porto, 4200-135 Porto, Portugal.; ³CNC – Center for Neuroscience and Cell Biology, 3004-504 Coimbra, Portugal.; ⁴ITQB – Instituto de Tecnologia Química Biológica, Universidade Nova de Lisboa, 2780-157 Oeiras, Portugal.; ⁵IIUC – Interdisciplinary Research Institute, University of Coimbra, 3004-504 Coimbra, Portugal.

External Resource:



MS-34a-1287-006_b.pdf

12:25pm - 12:45pm

Time-resolved serial femtosecond crystallography on photoswitchable fluorescent proteins

Kyprianos Hadjidemetriou

Institut de Biologie Structurale, Grenoble, France; kyprianos.hadjidemetriou@ibs.fr

External Resource:



MS-34a-491-007_b.pdf

MS-35: Polymorphism and structural transformation of organic crystals from synthesis to characterization

Location: **Club D**

Session Chair: **Kenneth D. M. Harris**

Session Chair: **Doris E. Braun**

Invited: **David Bryce (Canada), Franziska Emmerling (Germany)**

Introduction

10:20am - 10:25am

Introduction to session

10:20am - 12:45pm



MS-35-1766-001.pdf

10:25am - 10:55am

Preparation strategies and solid-state NMR characterization of supramolecular architectures based on halogen bonds, chalcogen bonds, and pnictogen bonds

David Bryce

University of Ottawa, Ottawa, Canada; dbryce@uottawa.ca

External Resource: Presentation



MS-35-139-002_b.pdf

10:55am - 11:25am

Mechanochemical cocrystal formation: Insights into polymorph control

Franziska Emmerling

Federal Institute for Materials Research and Testing, Berlin, Germany; franziska.emmerling@bam.de

External Resource: Presentation



MS-35-1141-003_b.pdf

11:25am - 11:45am

Pervasive approximate symmetry in organic P1 structures

Carolyn Pratt Brock

University of Kentucky, Lexington, United States of America; cpbrock@uky.edu

External Resource: Presentation



MS-35-1082-004_b.pdf

11:45am - 12:05pm

The Crystal Structure of Indomethacin Polymorph δ Solved by 3D Electron Diffraction

Molly Lightowler¹, Shuting Li², Xiao Ou², Xiaodong Zou¹, Ming Lu², Hongyi Xu¹

¹Department of Materials and Environmental Chemistry, Stockholm University, Stockholm SE-106 91, Sweden; ²School of Pharmaceutical Sciences, Sun Yat-sen University, Guangzhou 510006, China; molly.lightowler@mmk.su.se

External Resource: Presentation



MS-35-688-005_b.pdf

12:05pm - 12:25pm

Analysis of the experimental parameters impacting Non-Photochemical Laser-Induced nucleation of glycine in water

Nada Bosnjaković-Pavlović¹, Bertrand Clair¹, Aziza Ikni¹, Wenjing Li², Sladjana Novaković^{1,3}, Pascale Gemeiner¹, Philippe Scouffaire⁴, Anne Spasojević-de Biré¹

¹SPMS, Centralesupelec, Gif sur Yvette, France; ²BUCT Paris Curie Engineer School, Beijing, China; ³Institute of Nuclear Sciences, Vinca, Serbia; ⁴EM2C, Centralesupelec, Gif sur Yvette, France; anne.spasojevic@centralesupelec.fr

External Resource: Presentation



MS-35-1103-006_b.pdf

12:25pm - 12:45pm

Photo-induced electron transfer in Pyrene-(CH₂)₂-N,N'-Dimethylaniline: Time-resolved pink Laue X-ray diffraction studies on crystalline polymorphs.

Krishnayan Basuroy¹, Jose de J. Velazquez-Garcia¹, Darina Storozhuk¹, Robert Henning², David J. Gosztola³, Sreevidya Thekku Veedu¹, Simone Techert^{1,4}

¹Photon Science Division, Deutsches Elektronen-Synchrotron DESY, Hamburg, 22607, Germany; ²Center for Advanced Radiation Sources, The University of Chicago, Chicago, Illinois 60637, US.; ³Center for Nanoscale Materials, Argonne National Laboratory, Illinois 60439, US.; ⁴Institut für Röntgenphysik, Georg-August-Universität Göttingen, Göttingen, 37077, Germany; krishnayan.basuroy@desy.de

External Resource: Presentation



MS-35-1279-007_b.pdf

MS-36: Generalizations of crystallographic groups and their applications



Location: 221-2

Session Chair: **Gregory L McColm**

Session Chair: **Eden Delight Miro**

Invited: **Pavel Kalouguine (France), Martin Cramer Pedersen (Denmark)**

Introduction

10:20am - 10:25am

Introduction to session

Gregory L McColm, Eden Delight Miro



MS-36-1765-001.pdf

10:25am - 10:55am

Behind the curve: Generating and analysing nets and tessellations on periodic minimal surfaces in their universal covering space



Martin Cramer Pedersen¹, Jacob J. K. Kirkensgaard^{1,2}, Stephen T. Hyde³

¹Niels Bohr Institute, University of Copenhagen; ²Department of Food Science, University of Copenhagen; ³School of Chemistry, University of Sydney; mcpe@nbi.ku.dk

External Resource:



MS-36-726-002_b.pdf

10:55am - 11:25am

Flat-branched semisimplicial complexes: a versatile tool for aperiodic solids



Pavel Kalugin¹, André Katz²

¹Laboratoire de Physique des Solides, Université Paris-Saclay, Orsay, France; ²Directeur de recherche honoraire, CNRS, France; pavel.kalouguine@u-psud.fr

External Resource:



MS-36-1203-003_b.pdf

11:25am - 11:45am

Coordinated Colorings and their Chromatic Groups



Agatha Kristel M. Abila¹, Eduard C. Taganap², Ma. Louise Antonette N. De las Peñas³

¹Southern Luzon State University - Lucena Campus, Lucena City, 4301, Philippines; ²Department of Mathematics and Physics, Central Luzon State University, Science City of Munoz, Nueva Ecija 3120, Philippines; ³Department of Mathematics, Ateneo de Manila University, Quezon City, Metro Manila 1108, Philippines; agathakristelabila@gmail.com

External Resource:



MS-36-354-004_b.pdf

11:45am - 12:05pm

Advances in the application of magnetic and non-magnetic superspace-group symmetry



Branton J Campbell, Harold T Stokes

Brigham Young University, Physics & Astronomy, Provo, Utah, USA; branton@byu.edu

External Resource:



MS-36-978-005_b.pdf

12:05pm - 12:25pm

Magnetic modes compatible with the symmetry of crystals



Radosław Przeniosło, Piotr Fabrykiewicz, Izabela Sosnowska

University of Warsaw, Warsaw, Poland; radek@fuw.edu.pl

External Resource:



MS-36-1107-006_b.pdf

10:20am - 12:45pm

MS-37: Total scattering

Location: **Terrace 2A**

Session Chair: **Pierre Bordet**

Session Chair: **Emil Bozin**

Invited: **Stephan Rosenkranz (USA)**, **Bo Brummerstedt Iversen (Denmark)**

Introduction

10:20am - 10:25am

Introduction to session

Pierre Bordet, **Emil Bozin**



MS-37-1767-001.pdf

10:25am - 10:55am

Pair Distribution Function Analysis in Materials Science

Bo Brummerstedt Iversen

Aarhus University, Aarhus, Denmark; bo@chem.au.dk

External Resource:



MS-37-797-002_b.pdf

10:55am - 11:25am

Recent developments in measuring and analysing large 3D volumes of scattering data to investigate the role of complex disorder on crystalline materials properties

Stephan Rosenkranz, **Matthew J. Krogstad**, **Raymond Osborn**

Materials Science Division, Argonne National Laboratory, Lemont, Illinois 60439, United States of America; rosenkranz@anl.gov

External Resource:



MS-37-868-003_b.pdf

11:25am - 11:45am

Extracting interface correlations from the pair distribution function of composite materials

Harry S. Geddes¹, **Henry D. Hutchinson**¹, **Alex R. Ha**¹, **Nicholas P. Funnell**², **Andrew L. Goodwin**¹

¹Department of Chemistry, University of Oxford, South Parks Road, Oxford, OX1 3QR, U.K.; ²ISIS Facility, Rutherford Appleton Laboratory, Harwell Science and Innovation Campus, Didcot, OX11 0QX, U.K.; harold.geddes@chem.ox.ac.uk

External Resource:



MS-37-766-004_b.pdf

11:45am - 12:05pm

Total scattering at grazing incidence to study real thin film systems at variable temperature

Ann-Christin Dippel¹, **Olof Gutowski**¹, **Martin Roelsgaard**², **Bo B. Iversen**², **Marina Sturm**¹, **Martin v. Zimmermann**¹

¹Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany; ²Department of Chemistry, Aarhus University, 8000 Aarhus C, Denmark; ann-christin.dippel@desy.de

External Resource:



MS-37-1143-005_b.pdf

12:05pm - 12:25pm

Magnetic pair distribution function analysis of antiferromagnetic semiconductor MnTe

Parke Kip Hamilton, **Raju Baral**, **Jacob Christensen**, **Benjamin Frandsen**

Brigham Young University, Provo, United States of America; hami27@byu.edu

External Resource:



MS-37-976-006_b.pdf

12:25pm - 12:45pm

The local structure fingerprint of dual orbital degeneracy lifting in a strongly correlated electron system

Robert J. Koch¹, **Ryan Sinclair**², **Marshall T. McDonnell**³, **R. Yu**¹, **Milinda Abeykoon**⁴, **Matt Tucker**³, **Alexei M. Tsvelik**¹, **Simon J. L. Billinge**^{1,5}, **Haidong D. Zhou**², **Weiguo Yin**¹, **Emil S. Bozin**¹

¹Condensed Matter Physics and Materials Science Division, Brookhaven National Laboratory, Upton, NY 11973, USA; ²Department of Physics and Astronomy, University of Tennessee, Knoxville, TN 37996, USA; ³Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA; ⁴Photon Sciences Division, Brookhaven National Laboratory, Upton, NY 11973, USA; ⁵Department of Applied Physics and Applied Mathematics, Columbia University, New York, NY 10027, USA; rkoch@bnl.gov

External Resource:



MS-37-971-007_b.pdf

10:20am - 12:45pm

MS-38: Structural, electronic and magnetic ordering: From fundamental physics to functionality



Location: **Club C**

Session Chair: **Javier Sanchez-Benitez**

Session Chair: **Ovidiu Garlea**

Invited: **Christian Balz (USA)**, **Mark Senn (UK)**

Introduction

10:20am - 10:25am



Introduction to session

Javier Sanchez-Benitez, **Ovidiu Garlea**



MS-38-1768-001.pdf

10:25am - 10:55am

Magnetic Phase diagram of alpha-RuCl₃



Stephen Nagler, **Christian Balz**

Oak Ridge National Laboratory, Oak Ridge, United States of America; christian.balz@stfc.ac.uk

External Resource:



MS-38-1278-002_b.pdf

10:55am - 11:25am

Striping of orbital-order with charge-disorder in optimally doped manganites



Mark Senn

University of Warwick, Coventry, United Kingdom; m.senn@warwick.ac.uk

External Resource:



MS-38-1478-003_b.pdf

11:25am - 11:45am

Formation and ordering of orbital molecules in AV₂O₄ spinels



A. J. Browne^{1,2}, **J. P. Attfield**²

¹School of Chemistry, University of St Andrews, North Haugh, St Andrews KY16 9ST, United Kingdom; ²Centre for Science at Extreme Conditions and School of Chemistry, University of Edinburgh, West Mains Road, Edinburgh EH9 3FD, United Kingdom; ajb58@st-andrews.ac.uk

External Resource:



MS-38-877-004_b.pdf

11:45am - 12:05pm

Perovzalates: a family of perovskite-related oxalates



Rebecca Clulow^{1,2}, **Alasdair J. Bradford**^{2,3}, **Stephen L. Lee**³, **Philip Lightfoot**²

¹Department of Chemistry - Ångström Laboratory, Uppsala University, 751 21 Uppsala, Sweden; ²School of Chemistry, University of St Andrews, St Andrews, Fife, KY16 9ST, UK; ³School of Physics, University of St Andrews, St Andrews, Fife, KY16 9SS, UK; rebecca.clulow@kemi.uu.se

External Resource:



MS-38-472-005_b.pdf

12:05pm - 12:25pm

Aurivillius oxyfluorides: nuclear and magnetic order and the role of the anion sublattice



Emma E. McCabe

Durham University, Durham, United Kingdom; emma.mccabe@durham.ac.uk

External Resource:





MS-38-929-006_b.pdf

12:25pm - 12:45pm

Intermartensitic transformation between modulated structures in Heusler Ni-Mn-Ga-(Fe) single crystals

Oleg Heczko¹, Petr Veřtát^{1,2}, Milan Klicpera³, Oscar Fabelo⁴, Ladislav Straka^{1,3}

¹FZU - Institute of Physics of the Czech Academy of Sciences, Na Slovance 1999/2, 18221 Prague 8, Czech Republic; ²Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University in Prague, Trojanova 13, 12000 Prague 2, Czech Republic; ³Faculty of Mathematics and Physics, Charles University, Ke Karlovu 5, 12116 Prague 2, Czech Republic; ⁴Institut Laue-Langevin, 71 avenue des Martyrs, CS 20156, 38042 Grenoble cedex 9, France; heczko@fzu.cz

External Resource: Presentation



MS-38-1217-007_b.pdf

10:20am - 12:45pm

MS-39: Quantum crystallography in materials science

Location: **Terrace 2B**

Session Chair: **Simon Grabowsky**

Session Chair: **Jean-Michel Gillet**

Invited: **Rebecca Scatena (UK), Cherif Matta (Canada)**

Introduction

10:20am - 10:25am

Introduction to session

Simon Grabowsky, Jean-Michel Gillet



MS-39-1769-001.pdf

10:25am - 10:55am

Formate-mediated Magnetic Superexchange in the Model Hybrid Perovskite $[(CH_3)_2NH_2]Cu(HCOO)_3$: Applicability criteria for the GKA rules

Rebecca Scatena^{1,3}, Piero Macchi², Roger D. Johnson³

¹University of Oxford, Oxford, United Kingdom; ²Polytechnic of Milan, Milan, Italy; ³University College London, London, United Kingdom; rebecca.scatena@physics.ox.ac.uk

External Resource: Presentation



MS-39-349-002_b.pdf

10:55am - 11:25am

The Electric Field of ATP-Synthase

Jean-Nicolas Vigneau¹, Peyman Fahimi^{1,2}, Maximilian Ebert³, Youji Cheng^{2,4}, Chérif F. Matta^{2,4}

¹Département de chimie, Université Laval, Québec, QC, Canada G1V0A6; ²Department of Chemistry and Physics, Mount Saint Vincent University, Halifax, NS, Canada B3M2J6; ³Chemical Computing Group (CCG), Sherbrooke Street West, Montreal, QC, Canada H3A2R7; ⁴Department of Chemistry, Saint Mary's University, Halifax, NS, Canada B3H3C3; cherif.matta@msvu.ca

External Resource: Presentation



MS-39-1337-003_b.pdf

11:25am - 11:45am

Thermal stability of Glass forming Metal-Organic Framework: Role of metal-ligand bonding

Sounak Sarkar¹, Aref H. Mamakhei¹, Martin Bondesgaard¹, Hazel Reardon¹, Bo B. Iversen¹, Hidetaka Kasai², Eiji Nishibori²

¹Center for Materials Crystallography, Department of Chemistry and iNano, Aarhus University, Aarhus 8000, Denmark; ²Faculty of Pure and Applied Sciences, University of Tsukuba, 1-1-1 Tennodai, Tsukuba, Ibaraki 305-8571, Japan; sounaks@chem.au.dk

External Resource: Presentation



MS-39-819-004_b.pdf

11:45am - 12:05pm

Chemical bonding origin of the thermoelectric power factor in Half-Heusler semiconductors

Kasper Tolborg

Department of Materials, Imperial College London, Exhibition Road, London SW7 2AZ, United Kingdom; k.tolborg@imperial.ac.uk

External Resource: Presentation



MS-39-826-005_b.pdf

12:05pm - 12:25pm

Towards the measurement of bonding electron densities in nanostructured materials

Philip NH Nakashima¹, Xiaofen Tan¹, Ding Peng², Anna N Mortazavi^{3,4}, Laure Bourgeois^{1,5}, David R. Clarke³

¹Department of Materials Science, Monash University, Victoria 3800, Australia; ²Department of Physics, Norwegian University of Science and Technology (NTNU), Trondheim, Norway; ³School of Engineering and Applied Sciences, Harvard University, Cambridge, USA; ⁴Department of Physics, Chalmers University of Technology, Gothenburg, Sweden; ⁵Monash Centre for Electron Microscopy, Monash University, Victoria 3800, Australia.; philip.nakashima@monash.edu

External Resource:



MS-39-887-006_b.pdf

12:25pm - 12:45pm

Towards accurate positions of hydrogen atoms bonded to heavy metal atoms

Magdalena Wońska, Michał Chodkiewicz, Sylwia Pawłędzio, Krzysztof Wozniak

University of Warsaw, Warsaw, Poland; mwoinska@chem.uw.edu.pl

External Resource:



MS-39-557-007_b.pdf

MS-40: New applications of coherent scattering

Location: **223-4**

Session Chair: **Ian Robinson**

Session Chair: **Christian Gutt**

Invited: **Johanned Ihli** (Switzerland), **Foivos Perakis** (Sweden)

Introduction

10:20am - 10:25am

Introduction to session

Ian Robinson, **Christian Gutt**



MS-40-1770-001.pdf

10:25am - 10:55am

Molecular movies with X-ray photon correlation spectroscopy

Fivos Perakis

Physics Department, Stockholm University, Stockholm, Sweden; f.perakis@fysik.su.se

External Resource:



MS-40-1014-002_b.pdf

10:55am - 11:25am

Visualizing the effect additives have on the nanostructure of individual bio-inspired calcite crystal

Johannes Ihli¹, Yi-Yeoun Kim², Mark Levenstein², Yin Ning³, Klaus Wakonig¹, Mirko Holler¹, Steven Armes³, Ross Harder⁴, Ian Robinson⁵, Fiona Meldrum²

¹Paul Scherrer Institute, Villigen PSI, Switzerland; ²University of Leeds; ³University of Sheffield; ⁴Argonne National Laboratory;

⁵University College London; Johannes.ihli@psi.ch

External Resource:



MS-40-597-003_b.pdf

11:25am - 11:45am

Cateretê: The Coherent X-ray Scattering Beamline at the 4th generation synchrotron facility SIRIUS

Florian Meneau, Aline R Passos, Paulo RAF Garcia, Paloma Vinaches, Lais B Manoel, Tiago A Kalile, João P Zerba, Gustavo LMP Rodrigues, Eduardo Miqueles, Giovanni Baraldi, Jean Polli, Bernd C Meyer, Sergio AL Luiz, Carla Polo
Brazilian Synchrotron Light Laboratory (LNLS), Brazilian Center for Research in Energy and Materials (CNPEM);
florian.meneau@lnls.br

External Resource:



MS-40-1145-004_b.pdf

10:20am - 12:45pm

11:45am - 12:05pm

Burning cups and donuts: what coherent X-rays can reveal about topological defects

Dmitry Karpov¹, Justin Llandro², Edwin Fohntung³

¹European Synchrotron Radiation Facility, 71 Avenue des Martyrs, 38000 Grenoble, France; ²Tohoku University, Laboratory for Nanoelectronics and Spintronics, Sendai 980-8577, Japan; ³Department of Materials Science and Engineering, Rensselaer Polytechnic Institute, NY 12180 Troy, USA; dmitry.karpov@esrf.fr

External Resource:



MS-40-1060-005_b.pdf

12:05pm - 12:25pm

Coherent diffraction imaging at space-group forbidden reflections

Guillaume Beutier¹, Joel Eymery², Maxime Dupraz^{2,3}, Marie-Ingrid Richard^{2,3}, Alexis Wartelle^{1,3}, Marc Verdier¹, Marc de Boissieu¹, Steven P. Collins⁴, Ewen Bellec³, Vincent Favre-Nicolin³, Steven Leake³

¹SIMaP, CNRS / Grenoble INP / Univ Grenoble Alpes, France; ²CEA, IRIG, France; ³ESRF, France; ⁴Diamond Light Source, United Kingdom; guillaume.beutier@grenoble-inp.fr

External Resource:



MS-40-1302-006_b.pdf

12:25pm - 12:45pm

Machine Learning approach to the phase problem in Bragg Coherent Diffraction Imaging

Ian Robinson

University College, London, United Kingdom; i.robinson@ucl.ac.uk

External Resource:



MS-40-698-007_b.pdf

SMS-3: Online crystallography: Tools, apps and web services

Location: **Club H**

Session Chair: **Eugene Krissinel**

Session Chair: **Christian Bertram Hübschle**

Invited: **Mois Ilia Aroyo** (Spain), **Victor Lamzin** (Germany)

Introduction

10:20am - 10:25am

Introduction to session

Eugene Krissinel, **Christian Bertram Hübschle**



SMS-3-1837-001.pdf

10:20am - 12:45pm

10:25am - 10:55am

Symmetry database of International Tables online

Eli Kroumova¹, **Gemma de la Flor Martin**², **Nicola J. Ashcroft**³, **Mois Ilia Aroyo**⁴

¹eFaber Soluciones Inteligentes SL., Bilbao (Spain); ²Institute of Applied Geosciences, Karlsruhe Institute of Technology, Karlsruhe (Germany); ³Editorial Office, International Union of Crystallography, Chester (England); ⁴Departamento de Física, Universidad del País Vasco UPV/EHU, Bilbao (Spain); mois.aroyo@ehu.es

External Resource:



SMS-3-834-002_b.pdf

10:55am - 11:25am

Macromolecular Model Building Over the Web

Victor S. Lamzin, **Egor Sobolev**, **Philipp Heuser**

EMBL, Hamburg, Germany; victor@embl-hamburg.de



SMS-3-1535-003_b.pdf

11:25am - 11:45am

Live monitoring onsite, remote and unattended data collection on synchrotron MX beamlines

David Aragao, **Elliot Nelson**

Diamond Light Source, Harwell Science and Innovation Campus, Chilton, Didcot, OX11 0DE, UK; david.aragao@diamond.ac.uk

External Resource:





SMS-3-1213-004_b.pdf

11:45am - 12:05pm

Introduction to invariant-based machine learning for periodic crystals

Vitaliy Kurlin, Jakob Ropers, Marco M Mosca, Olga Anosova

University of Liverpool, Liverpool, United Kingdom; vitaliy.kurlin@liverpool.ac.uk

External Resource:



SMS-3-967-005_b.pdf



SMS-3-967-005_c.pdf

12:05pm - 12:25pm

Solving Macromolecular Structures Online with CCP4

Ville Uski, Eugene Krissinel, Charles Ballard, Andrey Lebedev, Ronan Keegan

Science and Technology Facilities Council, Didcot, United Kingdom; ville.uski@stfc.ac.uk

External Resource:



SMS-3-1435-006_b.pdf

12:25pm - 12:45pm

eSPC, an Online Data Analysis Platform for Molecular Biophysics

Maria m. Garcia Alai

EMBL, Hamburg, Germany; garcia@embl-hamburg.de

External Resource:



SMS-3-1872-007_b.pdf

ECA-ECM: ECM programme committees

Location: **Club H**

Session Chair: **Sylvain Ravy**

ECM programme committee meetings -Versaille,Padova

12:45pm - 2:45pm



Lunch 3: Exhibition, posters, lunches

Location: **Exhibition and poster area**

12:45pm - 2:45pm



Meeting 3 - Journals: Commission on Journals open meeting

Location: **Club A**

Session Chair: **Andrew Allen**

Session Chair: **Peter Raymond Strickland**

1:00pm - 2:00pm



CS-4: Commercial session - MiTeGen: Innovations in Crystallography and CryoEM

Location: **Terrace 2A**

Session Chair: **Milan Dopita**

30 min company presentation

video

1:30pm - 2:00pm



PL-1: How data have revealed the structural universe

Location: **Panorama**

Session Chair: **John Richard Helliwell**

Helen Berman

Video

2:50pm - 3:40pm



The data universe of structural biology

Helen Berman^{1,2}

¹Rutgers University, United States of America; ²University of Southern California, United States of America; berman@rcsb.rutgers.edu

External Resource:



PL-1-714-001_b.pdf

Bragg: W.H. and W.L. Bragg Prize

Location: **Panorama**

Session Chair: **Elena Boldyreva**

Prize - Lecture 1 - Lecture 2

3:45pm - 4:40pm



Structure-guided design of next-generation malaria vaccine

Jean-Philippe Julien

The Hospital for Sick Children, Toronto, Canada; jean-philippe.julien@sickkids.ca

External Resource:





Bragg-1013-001_b.pdf

Targeting COVID-19 Viral Enzymes in an Evolving Landscape of Publishing and Peer Review

James Fraser

UCSF, San Francisco, United States of America; jaimefraser@gmail.com

External Resource: Presentation



Bragg-1003-002_b.pdf

4:40pm - 5:40pm

Afternoon break 3: Poster session B1, exhibition, coffee/tea

Location: [Exhibition and poster area](#)

4:40pm - 5:40pm

Poster - 17 Biocrystallography: Macromolecular and biological crystallography

Poster session abstracts

Radomír Kužel



Poster - 17 Biocrystallography-1944-001.pdf

MyD88 TIR domain higher-order assembly interactions revealed by serial femtosecond crystallography

Susannah Holmes^{1,10}, Max T. B. Clabbers^{2,10,11}, Timothy W. Muusse³, Parimala R. Vajjhala³, Sara J. Thygesen³, Alpeshkumar K. Malde⁴, Dominic J. B. Hunter^{3,5,6}, Tristan I. Croll⁷, Leonie Flueckiger¹, Jeffrey D. Nanson³, Md. Habibur Rahaman³, Andrew Aquila⁸, Mark S. Hunter⁸, Mengning Liang⁸, Chun Hong Yoon⁸, Jingjing Zhao², Nadia A. Zatsepin¹, Brian Abbey¹, Emma Sieracki⁵, Yann Gambin⁵, Katryn J. Stacey^{3,6,9}, Connie Darmanin¹, Bostjan Kobe^{3,6,9}, Hongyi Xu², Thomas Ve⁴

¹Australian Research Council Centre of Excellence in Advanced Molecular Imaging, Department of Chemistry and Physics, La Trobe Institute for Molecular Science, La Trobe University, Melbourne, Victoria, Australia; ²Department of Materials and Environmental Chemistry, Stockholm University, Stockholm, Sweden; ³School of Chemistry and Molecular Biosciences, The University of Queensland, Brisbane, Queensland, Australia; ⁴Institute for Glycomics, Griffith University, Southport, Queensland, Australia; ⁵EMBL Australia Node in Single Molecule Science, University of New South Wales, Kensington, New South Wales, Australia; ⁶Institute for Molecular Bioscience, The University of Queensland, Brisbane, Queensland, Australia; ⁷Cambridge Institute for Medical Research, University of Cambridge, Cambridge, UK; ⁸Linac Coherent Light Source, SLAC National Accelerator Laboratory, Menlo Park, California, USA; ⁹Australian Infectious Diseases Research Centre, The University of Queensland, Brisbane, Queensland, Australia; ¹⁰These authors contributed equally: Susannah Holmes, Max T. B. Clabbers; ¹¹Present address: Department of Biological Chemistry, University of California Los Angeles, Los Angeles, California, USA; susannahholmes@gmail.com

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Poster - 17 Biocrystallography-1469-002_b.pdf

Crystal structure of atypical ubiquitin ligase PCAF_N

Sachiko TOMA-FUKAI¹, Ryota HIBI², Takao NAGANUMA³, Mashito SAKAI³, Shinya SAIJO⁴, Nobutaka SHIMIZU⁴, Michihiro MATSUMOTO³, Toshiyuki SHIMIZU²

¹Nara Institute of Science and Technology; ²The University of Tokyo; ³National Center for Global Health and Medicine; ⁴High Energy Accelerator Research Organization (KEK)

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Poster - 17 Biocrystallography-1452-003_b.pdf

Structural characterization of seven-bladed beta-propeller lectin family from *Photobacterium laumondii*

Eva Fajdová^{1,2}, Josef Houser^{1,2}, Filip Melicher², Michaela Wimmerová^{1,2,3}

¹National Centre for Biomolecular research, Masaryk University, Brno, Czech Republic; ²Central European Institute of Technology, Brno, Czech Republic; ³Department of Biochemistry, Faculty of Science, Masaryk University, Brno, Czech Republic

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Structural study of the inhibitory mechanism of tau recognition antibody to tau aggregation

Tomohiro Tsuchida¹, Takahiro Tsuchiya¹, Katsushiro Miyamoto¹, Shinji Takai¹, Teruo Ueno¹, Yoshihiko Fujioka¹, Yasuko In¹, Katsuhiko Minoura¹, Taizo Taniguchi², Koji Tomoo¹

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Molecular-biology and structural study of Avian orthoreovirus non-structural proteins

Barbora Kaščáková¹, Zdenek Franta¹, Zdeno Gardian^{1,2}, Ivana Kutá Smatanová¹, Roman Tůma^{1,3}

¹University of South Bohemia in České Budějovice, České Budějovice, Czech Republic; ²Biology Centre CAS, Laboratory of electron Microscopy, Ceske Budejovice, Czech Republic; ³University of Leeds, School of Molecular and Cellular Biology, The Astbury Centre for Structural Molecular Biology, Leeds, UK

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Surface Layer Proteins of *Lactobacillus acidophilus* - A Story of SlpA and SlpX

Theo Sagmeister¹, Markus Eder¹, Christoph Grininger¹, Christoph Buhlheller¹, Đjenana Vejzović¹, Andela Đordić¹, Elisabeth Damisch¹, Claudia Millán², Isabel Usón³, Tea Pavkov-Keller^{1,4,5}

¹Institute of Molecular Biosciences, University of Graz, Austria; ²Structural Biology, Crystallographic Methods group at IBMB-CSIC, Barcelona; ³Structural Biology, ICREA at IBMB-CSIC, Barcelona; ⁴BioTechMed, Graz; ⁵Field of Excellence BioHealth, University of Graz, 8010 Graz, Austria

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Structural characterization of the PTG and PTG/PP1 complex

Marta Stefania Semrau^{1,2}, Graziano Lolli¹, Paola Storici², Gabriele Giachin³, Sonia Covaceuszach⁴

¹University of Trento, Department of Cellular, Computational and Integrative Biology (CIBIO), Trento, Italy; ²Protein Facility, Elettra Sincrotrone Trieste S.C.p.A, Italy; ³University of Padova, Department of Chemical Sciences (DiSC), Padova, Italy; ⁴CNR – Institute of Crystallography, Trieste, Italy

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OrfG, a VirB8-like protein encoded by an integrative and conjugative element in *S. thermophilus*, has a trimeric architecture with intertwined subunits that may be involved in the Gram-positive Conj-T4SS.

Julien Cappelle¹, Badreddine Douzi², Sandrine Mathiot¹, Nathalie Leblond-Bourget², Claude Didierjean¹, Frédérique Favier¹

¹CRM², Nancy, France; ²Université de Lorraine, INRAE, DynAMic, Nancy, France; julien.cappelle@univ-lorraine.fr

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A solution-free crystal-mounting platform for native SAD

Jian Yu, Akira Shinoda, Koji Kato, Isao Tanaka, Toyoyuki Ose, Min Yao

Faculty of Advanced Life Science, Hokkaido University, Sapporo, Japan; yu@castor.sci.hokudai.ac.jp

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Structural insights into the phlorotannin binding of EHEP and akuBGL for producing biofuel from brown algae

xiaomei sun¹, Yuxin Ye¹, Naofumi Sakurai¹, Koji Kato¹, Jian Yu¹, Keizo Yuasa², Akihiko Tsuji², Min Yao¹

¹Faculty of Advanced Life Science, Hokkaido university; ²Graduate School of Bioscience and Bioindustry, Tokushima University

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Structural studies of C-reactive Protein

Stacey Marie Collister, William Neale, Jamie Littlejohn, Trevor Greenhough, Annette Shrive

Keele University, Staffordshire, United Kingdom; s.collister@keele.ac.uk

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Poster - 17 Biocrystallography-1533-012_c.pdf

Structural studies of bacterial small alarmone hydrolases

Adriana Chrenková, Francesco Bisiak, Ditlev Egeskov Brodersen
Aarhus University, Aarhus, Denmark

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Investigation of possible tolerance mutations in a VapBC Toxin-Antitoxin system through structure determination

Maria Raadkjær Nielsen, Ditlev Egeskov Brodersen
Department of Molecular Biology and Genetics, Aarhus University, Gustav Wieds Vej 10, DK-8000, Aarhus C, Denmark

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Poster - 17 Biocrystallography-1697-014_b.pdf

Investigations on *Vibrio cholerae* sensory regulator ToxR

Nina Gubensäk, Gabriel E. Wagner, Evelyne Schrank, Fabio S. Falsone, Tamara Margot Ismael Berger, Joachim Reidl, Klaus Zangger, Tea Pavkov-Keller
University of Graz, Graz, Austria; nina.gubensaek@uni-graz.at

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Poster - 17 Biocrystallography-1665-015_b.pdf



Poster - 17 Biocrystallography-1665-015_c.pdf

FAD-dependent oxidoreductase from *Chaetomium thermophilum*: Crystallographic fragment screening-based identification of putative substrates

Leona Švecová^{1,2}, Lars Henrik Østergaard³, Tereza Skálová¹, Tomáš Kovar¹, Jan Dohnálek¹

¹Institute of Biotechnology of the Czech Academy of Sciences, v.v.i., Průmyslová 595, 252 50 Vestec, Czech Republic; ²Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University in Prague, Břehová 7, 115 19 Prague 1, Czech Republic;

³Novozymes A/S, Biologiens Vej 2, 2800 Kgs. Lyngby, Denmark,

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Structure-assisted design of inhibitors of CA IX enzyme based on polyhedral boron compounds

Jiří Brynda^{1,4}, Michael Kugler^{1,4}, Jan Nekvinda², Josef Holub², Suzan El Anwar², Wiswanath Das³, Václav Šícha², Klára Pospíšilová¹, Milan Fábry⁴, Vlastimil Král⁴, Petr Pacht¹, Marián Hajdúch³, Bohumír Grüner², Pavlína Řezáčová^{1,4}

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Poster - 17 Biocrystallography-1857-017_c.pdf

Understanding the structural and functional aspects of a novel Mg²⁺-citrate-binding protein

Suraj Kumar Mandal, Shankar Prasad Kanaujia

Department of Biosciences and Bioengineering, Indian Institute of Technology Guwahati, India, Guwahati, India;
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MlaC represents a unique class of solute-binding proteins

Angshu Dutta, Shankar Prasad Kanaujia

Department of Biosciences and Bioengineering, Indian Institute of Technology Guwahati (IITG), Guwahati, India;
angshudutta39@iitg.ac.in

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Evolutionary upgrade of stefins for secretion in parasites

Michal Buša¹, Zuzana Matoušková¹, Pavlína Řezáčová¹, Pavla Sojková-Bartošová², Martin Horn¹, Saša Štefanič³, Michael Mareš¹

¹Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences, Flemingovo nám. 2, Prague, 166 10, Czechia;

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Poster - 17 Biocrystallography-1885-020_b.pdf

Light-induced oligomerization of the transcription factor EL222

Aditya S. Chaudhari¹, Edel Cunill Semanat¹, Anne Martel², Bohdan Schneider¹, **Gustavo Fuenes**¹

¹Institute of Biotechnology CAS v.v.i., Vestec, Czech Republic; ²Institut Laue-Langevin, Grenoble, France; gustavo.fuenes@ibt.cas.cz



Poster - 17 Biocrystallography-1868-021_b.pdf

Poster - 18 CryoEM: Cryo-EM

Session Chair: Jose-Maria Carazo

Session Chair: Jiri Novacek



4:40pm - 5:40pm

Poster session abstracts

Radomír Kužel



Poster - 18 CryoEM-1945-001.pdf

Structural analysis of transcription related complexes and operation of 200kV cryo-EM in KEK

Naruhiko Adachi, Masato Kawasaki, Toshio Moriya, Akira Shinoda, Yusuke Yamada, Toshiya Senda

High Energy Accelerator Research Organization (KEK), Ibaraki, Japan



Poster - 18 CryoEM-168-002_b.pdf

SAMase of bacteriophage T3 inactivates E. coli's methionine Sadenosyltransferase by forming hetero-polymers

Hadas Simon-Baram¹, Daniel Kleiner¹, Fannia Shmulevich¹, Raz Zarivach^{1,2}, Ran Zalk², Huayuan Tang³, Feng Ding³, Shimon Bershtein¹

¹Department of Life Sciences, Ben-Gurion University of the Negev, Beer-Sheva, Israel; ²Macromolecular Crystallography and Cryo-EM Research Center, The National Institute for Biotechnology in the Negev, Ben-Gurion University of the Negev, Beer-Sheva, Israel;

³Department of Physics and Astronomy, Clemson University, Clemson, South Carolina, USA

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Poster - 18 CryoEM-1456-003_b.pdf

Reciprocal space refinement and map calculation for cryo-EM single particle structures

Keitaro Yamashita, Rangana Warshamanage, Garib N. Murshudov

MRC Laboratory of Molecular Biology, Cambridge, United Kingdom; kyamashita@mrc-lmb.cam.ac.uk

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Poster - 18 CryoEM-1238-004_b.pdf

Cryo-EM structure of a functional monomeric Photosystem I from Thermosynechococcus elongatus reveals red chlorophyll cluster

Christoph Gerle¹, Orkun Coruh², Anna Frank³, Hideaki Tanaka², Akihiro Kawamoto², Eithar El-Mohsawy⁴, Takayuki Kato², Keiichi Namba², Marc Nowaczyk³, Genji Kurisu²

¹Riken, Sayo, Japan; ²Osaka University, Japan; ³Ruhr Universität Bochum, Germany; ⁴Kafrelsheikh University, Egypt

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Poster - 18 CryoEM-1415-005_b.pdf

Structural Comparison of heterotrimer PCNA from Crenarchaeon *Aeropyrum pernix* by solution scattering, Cryo-EM, and Crystallography

Takahiro Yamauchi^{1,2}, Tsubasa Takemori³, Makiko Kikuchi⁴, Yasuhito Iizuka^{1,3}, Satoshi Ishikawa³, Masaru Tsunoda^{1,3,4}

¹Grad. Sch. of Life Sci. and Tech., Iryo Sosei Univ.; ²Dept. of Pharm., Fukushima Rosai Hosp.; ³Fac. of Pharm., Iryo Sosei Univ.;

⁴Grad. Sch. of Sci. and Eng., Iryo Sosei Univ.

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Poster - 18 CryoEM-1499-006_b.pdf

Structural analysis of a tetradecameric HSP100 chaperone by cryo-EM and SAXS

Hyunwoo Cho, Gyuhee Kim, Sangho Lee

SungKyunKwan University, Suwon, Korea, Republic of (South Korea); gusdnf0326@naver.com

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Poster - 18 CryoEM-1506-007_b.pdf

Developments in Advanced Handling, Storage, Transport, and Tracking of Cryo-EM Samples

Benjamin Apker, David Closs, Robert Thorne, Rich Jayne

MiTeGen LLC, Ithaca, United States of America; benjamin.apker@mitegen.com

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Poster - 18 CryoEM-1842-008_b.pdf

Cryo-electron tomography study of detonation nanodiamonds hydrosols

Alexey A. Mikhutkin¹, Roman A. Kamyshinsky^{1,2}, Nikita M. Kuznetsov¹, Sergei N. Chvalun¹, Alexander L. Vasiliev^{1,2}

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Poster - 18 CryoEM-451-009_b.pdf

Poster - 19 Pharmaceutical: Pharmaceutical materials

Session Chair: **Nikoletta B. Bathori**

Session Chair: **Laszlo Fabian**

Comment

Poster session abstracts

Radomír Kužel



Poster - 19 Pharmaceutical-1946-001.pdf

New salts of levofloxacin with physicochemical, structural and biological insights

Mayank Joshi¹, Indu Verma¹, Aakanksha Gulati², Susmita Rani³, Chesta Budhwar⁴, Kaiser Raza⁵, Arunika Mukhopadhyaya², Angshuman Roy Choudhury¹

¹Department of Chemical Sciences, Indian Institute of Science Education and Research, Mohali, Sector 81, S. A. S. Nagar, Knowledge City, Manauli P. O. Mohali, Punjab, India-140306; ²Department of Biological Sciences, Indian Institute of Science Education and Research, Mohali, Sector 81, S. A. S. Nagar, Knowledge City, Manauli P. O. Mohali, Punjab, India-140306; ³MCM DAV College for Women, Sector 36, Chandigarh, U. T., India-160036; ⁴Department of Chemistry, Indian Institute of Technology, Jodhpur, N.H. 65, Karwar, Rajasthan, India-342037; ⁵Department of Pharmacy, School of Chemical Sciences and Pharmacy, Central University of Rajasthan, Bandarsindri, Dist. Ajmer, Rajasthan, India-305817; mayankjoshi@iiser-mohali.ac.in

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Poster - 19 Pharmaceutical-142-002_b.pdf

Pharmaceutical cocrystallization: polymorphs, salts and cocrystals

Angshuman Roy Choudhury¹, Maheswararao karanam¹, Mayank Joshi¹, Indu Verma¹, Aakanksha Gulati², Chesta Budhwar³, Sushmita Rani⁴, Aanchal Bhalla⁴, Pooja Garg⁵, Arunika Mukhopadhyay², Kaiser Raza⁶, Dev Sagarika⁴

4:40pm - 5:40pm



¹Department of Chemical Sciences, Indian Institute of Science Education and Research Mohali, Mohali, India; ²Department of Biological Sciences, Indian Institute of Science Education and Research, Mohali, Sector 81, S. A. S. Nagar, Manauli PO, Mohali, Punjab, India. 140306; ³Department of Chemistry, Indian Institute of Technology, Jodhpur, N.H. 65, Karwar, Rajasthan; ⁴MCM DAV College for Women, Sector 36, Chandigarh, Union Territory, India. 160036; ⁵Post Graduate Government College, Chandigarh, Union Territory, India. 160011; ⁶Department of Pharmacy, School of Chemical Sciences and Pharmacy, Central University of Rajasthan, Bandarsindri, Dist. Ajmer, Rajasthan, India. 305817; angshurc@iisermohali.ac.in

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Poster - 19 Pharmaceutical-164-003_b.pdf

3D Electron diffraction for the discovery of new crystal forms of APIs

Arianna E. Lanza¹, Jason Potticary², Charlie Hall², Victoria Hamilton², Simon R. Hall², Gustavo Santiso-Quinones¹, Gunther Steinfeld¹, Eric Hovestreydt¹

¹ELDICO Scientific AG, 5234 Villigen, Switzerland; ²School of Chemistry, University of Bristol, Cantock's Close, Bristol, BS8 1TS, United Kingdom; lanza@eldico.ch

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Poster - 19 Pharmaceutical-829-004_b.pdf

Crystal growth and optical study of thalidomide

Mizuki Kira¹, Koichi Tsutao¹, Kun Zhang¹, Yukana Terasawa¹, Norio Shibata², Toru Asahi³

¹Waseda University, Shinjuku-ku, Japan; ²Graduate School of Engineering, Nagoya Institute of Technology, Nagoya, Japan;

³Research Organization for Nano and Life Innovation, Waseda University, Shinjuku-ku, Japan; kira5-5@akane.waseda.jp

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Poster - 19 Pharmaceutical-1316-005_b.pdf

Synthesis and characterization of metallo-drugs with potential use for overweight treatment

Richard Fernando DVries, Stephanny Villamizar-Delgado, Octavio Piñeros, Javier Ellena

Universidad Santiago de Cali, Cali, Colombia; richard.dvries00@usc.edu.co

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Poster - 19 Pharmaceutical-624-006_b.pdf

Effect of grinding procedures on the ritonavir-lopinavir system

Lucas B. M. Pinheiro¹, Elizabeth Culbertson², Gabriel L. B. de Araujo³, Simon Billinge², Fabio Furlan Ferreira^{1,4}

¹Center for Natural and Human Sciences (CCNH), Federal University of ABC (UFABC), Santo André, Brazil; ²Columbia University, New York, USA; ³University of São Paulo, São Paulo, SP, Brazil; ⁴Nanomedicine Research Unit (NANOMED), Federal University of ABC (UFABC), Santo André, SP, Brazil; fabio.furlan@ufabc.edu.br

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Poster - 19 Pharmaceutical-944-007_b.pdf

Chaperone Compounds for Co-crystallization of Organics

Fabian Rami¹, Tobias Stuerzer², Clemens Richert¹, Martin Adam²

¹Universität Stuttgart, Institut für Organische Chemie, Stuttgart, Germany; ²Bruker AXS GmbH, Karlsruhe, Germany; Martin.Adam@bruker.com

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The "Molecular Grabber" method: Development of another crystalline sponge New idea for structure analysis of compounds using protein

Takashi Matsumoto¹, Akihito Yamano¹, Ryosuke Nakashima², Kunihiro Nishino²

¹Rigaku Corporation; ²Institute of Scientific and Industrial Research, Osaka University; t-matsumo@rigaku.co.jp

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An unexpected and unusually complex Co-Mefenamate with nine octahedrally coordinated crystallographically independent cobalt atoms obtained at room temperature

Graciela C. Díaz de Delgado¹, Manuel E. Vivas-Arellano¹, Robert A. Toro Hernández², José Antonio Henao Martínez², José Miguel Delgado Quiñones¹

¹Laboratorio de Cristalografía-LNDRX, Departamento de Química, Facultad de Ciencias, Universidad de Los Andes, Mérida, Venezuela; ²Grupo de Investigación en Química Estructural (GIQUE), Escuela de Química, Facultad de Ciencias, Universidad Industrial de Santander, Bucaramanga, Colombia; gdiazdedelgado@gmail.com

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Poster - 19 Pharmaceutical-1671-010_b.pdf

Nitroxide with diphenylphosphino moiety: synthesis, supramolecular structure, biology and catalysis

Attila Csaba Benyei¹, Mostafa Isbera², Balázs Bognár², Ferenc Gallyas^{3,4,6}, József Jekő⁵, Tamás Kálai²

¹University of Debrecen Department of Pharmaceutical Chemistry; ²University of Pécs Institute of Organic and Medicinal Chemistry; ³University of Pécs Department of Biochemistry and Medical Chemistry; ⁴HAS-UP Nuclear-Mitochondrial Interactions Research Group Budapest; ⁵University of Nyíregyháza Department of Chemistry; ⁶University of Pécs János Szentágotthai Research Center; benyei.attila@science.unideb.hu

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Poster - 19 Pharmaceutical-1722-011_b.pdf

New forms of pharmaceutical co-crystals of gefitinib with resorcinol

Parimaladevi Palanisamy

University of Limerick, Castletroy, Ireland; p.palanisamy@ul.ie

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Poster - 19 Pharmaceutical-1699-012_b.pdf

Study in the Solid State, Framework Energy and Crystal Structure by X-Ray Diffraction Techniques of Cetirizine and Levocetirizine Dihydrochloride Used as an Antihistamines

Angie Paola Tamayo Carreño, Robert Antonio Toro Hernández, José Antonio Henao Martínez

Grupo de Investigación en Química Estructural, Universidad Industrial de Santander, Bucaramanga, Colombia; angietamayocarreno@gmail.com

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Poster - 19 Pharmaceutical-331-013_b.pdf

Influence of guest lattice solvents on nanomechanical properties of pharmaceutical crystalline solids

Subhrajyoti Bhandary^{1,2}, Pradip Kumar Mondal², S. R. N. Kiran Mangalampalli³, Upadrasta Ramamurthy⁴, Deepak Chopra²

¹Department Of Chemistry, Ghent University, Belgium; ²Department Of Chemistry, INDIAN INSTITUTE OF SCIENCE EDUCATION BHOPAL, India; ³Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur, India; ⁴School of Mechanical and Aerospace Engineering, Nanyang Technological University, Singapore; subhrajyoti.bhandary@ugent.be

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Photoswitchable dismantlers of biomaterials made of amyloid fibrils.

Przemysław Kozminski¹, Krzysztof Lyczko¹, Zuzana Bednarikova², Zuzana Gazova², Imola Wilhelm³, Istvan Krizbai³, Grzegorz Wieczorek⁴, Dorota Niedzialek⁴

¹Institute of Nuclear Chemistry and Technology, Warsaw, Poland; ²Institute of Experimental Physics, Slovak Academy of Sciences, Kosice, Slovakia; ³Institute of Biophysics, Biological Research Center, Hungarian Academy of Sciences, Szeged, Hungary; ⁴Institute of Biochemistry and Biophysics Polish Academy of Sciences, Warsaw, Poland; dniedzialek@ibb.waw.pl

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Poster - 19 Pharmaceutical-1686-015_b.pdf

Poster session abstracts

Radomír Kužel

Poster - 20 Polymorphism-1947-001.pdf

Importance of Polymorphism in Improving the Potency of Bioactive Molecules

ANIL KUMAR, Jyoti Chauhan, Kshatresh Dutta Dubey, Subhabrata Sen, Parthapratim Munshi*Shiv Nadar University, Greater Noida, India; ak803@snu.edu.in

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Poster - 20 Polymorphism-498-002_b.pdf

Tunable temperature of reversible phase transitions in a series of heterometallic carboxylate complexes with CaZn₂-backboneStanislav Nikolaevich Melnikov, Stanislav Alexandrovich Nikolaevskii, Mikhail Alexandrovich Kiskin, Igor Leonidovich EremenkoIGIC RAS, Moscow, Russian Federation; stas_melnikov_1@mail.ru

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Poster - 20 Polymorphism-647-003_b.pdf

Structural analysis, Ferroelectric and dielectric properties of single component organic multifunctional materials

REKHA KUMARI, T. N. Guru RowINDIAN INSTITUTE OF SCIENCE, Bangalore, India; rekhakumari@iisc.ac.in

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Poster - 20 Polymorphism-992-004_b.pdf

Stacking differences and similarities between a new and two old lapachol polymorphs

Natasha Di Benedetto¹, Miguel Ángel Martínez-Cabrera², Mario Alberto Macías³, Javier Enrique Barúa⁴, Leopoldo Suescun¹¹Cryssmat-Lab, DETEMA, Facultad de Química, Universidad de la República, Av. Gral Flores 2124, Montevideo 11800, Uruguay;²Universidad Nacional de Asunción, Facultad de Ciencias Exactas y Naturales, Departamento de Biología, Área Química Orgánica deProductos Naturales-LAREV, San Lorenzo Campus-UNA, Paraguay; ³Department of Chemistry, Universidad de los Andes, Cra. 1 N°18A-12, 111711, Bogotá, Colombia; ⁴Universidad Nacional de Asunción, Facultad de Ciencias Químicas, San Lorenzo Campus-UNA,Paraguay; ndibenedetto@fq.edu.uy

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Poster - 20 Polymorphism-279-005_b.pdf

Synthesis & crystallographic, spectroscopic and computational characterization of O-R substituents effects on the torsional angle of 3,3',4,4' substituted biphenyls

Nahir Vadra¹, Leonardo D. Slep¹, Veronica E. Manzano¹, Emilia B. Halac², Ricardo F. Baggio², Sebastian A. Suarez¹, Fabio D. Cukiernik¹¹University of Buenos Aires, CABA, Argentine; ²National Atomic Energy Commission, Argentine; vadra@qi.fcen.uba.ar

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Poster - 20 Polymorphism-186-006_b.pdf

A difficult art of crystallizing and characterizing elusive polymorphs of meloxicam

Justyna Śniechowska, Piotr Paluch, Marta K. DudekCenter of Molecular and Macromolecular Studies, Polish Academy of Sciences, Lodz, Poland; mdudek@cmm.lodz.pl

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Poster - 20 Polymorphism-1051-007_b.pdf

The phenomenon of polymorphism within the stereoatomic model of crystal structures

Anton V. Savchenkov, Viktor N. Serezhkin

Samara National Research University, Samara, Russian Federation; anton.savchenkov@gmail.com

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Poster - 20 Polymorphism-1202-008_b.pdf

Crystal and molecular structures of small-molecule solids solved with the free-distribution software PSSP and WinPSSP

Silvina Pagola¹, Alekos Polymeros², Nikolaos Kourkouvelis²

¹Old Dominion University, Williamsburg, United States of America; ²University of Ioannina, Ioannina, Greece; spagola@odu.edu

External Resource:



Poster - 20 Polymorphism-389-009_b.pdf

Influence of the Lewis basicity hardness of recrystallization solvents on the coordination sphere of the complex [Co(3,5-dinitrobenzoate-O,O')₂].

Andrés Felipe Pérez, Daniela Fonseca, John Jady Hurtado, Mario Alberto Macías

Universidad de los Andes, Bogota, Colombia; af.perez10@uniandes.edu.co

External Resource:



Poster - 20 Polymorphism-555-010_b.pdf

Determination of the crystal structure of magnesium stearate hydrate using micrometre size single crystals

Toms Rekis¹, Mikkel Herzberg¹, Anders Støttrup Larsen¹, Ana Gonzalez², Jukka Rantanen¹, Anders Østergaard Madsen¹

¹Department of Pharmacy, University of Copenhagen, Universitetsparken 2, 2100 København Ø, Denmark; ²MAX IV Laboratory, Lund University, PO Box 118, SE-221 00 Lund, Sweden; toms.rekis@sund.ku.dk

External Resource:



Poster - 20 Polymorphism-1532-011_b.pdf

Poster - 21 Quantum: Quantum crystallography

Session Chair: **Chérif F. Matta**

Session Chair: **Anna Maria Makal**

Session Chair: **PIERO MACCHI**

Session Chair: **Katarzyna N. Jarzemska**



4:40pm - 5:40pm

Poster session abstracts

Radomír Kužel



Poster - 21 Quantum-1948-001.pdf

How flexible is the water molecule structure? Cambridge Structural Database and *ab initio* calculations study.

Milan R. Milovanović¹, Jelena M. Živković¹, Dragan B. Ninković¹, Ivana M. Stanković², Snežana D. Zarić^{3,4}

¹Innovation center of the Faculty of Chemistry, Studentski trg 12-16, Belgrade, 11000, Serbia; ²Institute of Chemistry, Technology and Metallurgy, University of Belgrade, Njegoševa 12, 11000 Belgrade, Serbia; ³Faculty of Chemistry, University of Belgrade, Studentski trg 12-16, Belgrade, 11000, Serbia; ⁴Texas A&M University at Qatar, Education City, PO Box 23874, Doha, Qatar; milovanovic@chem.bg.ac.rs

External Resource:



Poster - 21 Quantum-448-002_b.pdf

Crystallographic and Computational Electron Density of d_{x2-y2} Orbitals of Azo-Schiff Base Metal Complexes Using Conventional Programs

Yuji Takiguchi, Takashi Akitsu

Tokyo University of Science, Shinjuku-ku, Japan; 1321574@ed.tus.ac.jp

External Resource:



Poster - 21 Quantum-1384-003_b.pdf

EVIDENCE OF STRONG HYDROGEN BONDING IN CRYSTAL STRUCTURES OF TRANSITION METAL COMPLEXES

Danijela S. Kretić, Dušan Ž. Veljković, Snežana D. Zarić

Faculty of Chemistry, University of Belgrade, Belgrade, Serbia; danijela@chem.bg.ac.rs

External Resource:



Poster - 21 Quantum-468-004_b.pdf

Computational analysis of intermolecular interactions in a crystal with structural phase transitions

Daisuke Takagi¹, Toru Asahi^{1,2}, Takuya Taniguchi³

¹Graduate School of Advanced Science and Engineering, Waseda University, 3-4-1 Okubo, Shinjuku-ku, Tokyo, Japan; ²Research Organization for Nano & Life Innovation, Waseda University, 513 Waseda-tsurumakicho, Shinjuku-ku, Tokyo, Japan; ³Center for Data Science, Waseda University, 1-6-1 Nishi-waseda, Shinjuku-ku, Tokyo, Japan; daichan.t@fuji.waseda.jp

External Resource:



Poster - 21 Quantum-1385-005_b.pdf

The benefit and challenges of non-spherical refinements – *NoSpherA2*

Florian Kleemiss¹, Simon Grabowsky², Oleg V. Dolomanov³, Horst Puschmann³, Michael Bodensteiner¹

¹University of Regensburg, Department for Chemistry and Pharmacy, Universitätsstraße 31, 93053 Regensburg, Germany; ²University of Bern, Department of Chemistry, Biochemistry and Pharmacy, Freiestrasse 3, 3012 Bern, Switzerland; ³OlexSys Ltd., Chemistry Department, Durham University, DH1 3LE, United Kingdom; florian.kleemiss@ur.de

External Resource:



Poster - 21 Quantum-1147-006_b.pdf

Charge density distribution of API in crystals and ligand-receptor complexes

Alexander A. Koriyukov¹, Anna V. Vologzhanina¹, Adam I. Stash¹, Krzysztof Wozniak²

¹A. N. Nesmeyanov Institute of Organoelement Compounds, RAS, 28 Vavilova str, 119991 Moscow, Russia; ²Biological and Chemical Research Centre, Department of Chemistry, University of Warsaw, Żwirki i Wigury 101, 02089 Warsaw, Poland; alex@xrlab.ineos.ac.ru



Poster - 21 Quantum-1075-007_b.pdf

Intermolecular interaction analysis from SCXRD and their relationship with observed properties in potential pharmaceuticals

Natalia Alvarez¹, Antonio José Costa-Filho², Javier Ellena³, Gianella Facchin¹

¹Facultad de Química, Universidad de la República, Montevideo, Uruguay; ²Faculdade de Filosofia, Ciências e Letras de Ribeirão Preto, Universidade de São Paulo, SP, Brazil; ³Instituto de Física de São Carlos, Universidade de São Paulo, SP, Brazil; nalvarez@fq.edu.uy

External Resource:



Poster - 21 Quantum-542-008_b.pdf

Three-Dimensional topological analysis of the experimental and theoretical electron density of a 5-Fluorocytosine/Isoniazid cocrystal

Adilson Barros Wanderley¹, Juan Carlos Tenorio², Ihosvany Camps³, Christian W. Lehmann⁴, Javier Ellena¹

¹Instituto de Física de São Carlos - USP, C.P. 369, 13560-970, São Carlos, SP, Brazil; ²Instituto de Química, Universidade Estadual de Campinas - Unicamp, CEP 13083-970, Campinas, SP, Brazil; ³Departamento de Física, ICEx/UNIFAL-MG, Alfenas, MG, 37133-840, Brazil; ⁴Max-Planck-Institut für Kohlenforschung, 45470, Mülheim a.d Ruhr, Germany; javiere@ifsc.usp.br

External Resource:



Poster - 21 Quantum-402-009_b.pdf

Quantum crystallography, spectroscopic methods, and hot stage microscopy in the study of chromic multicomponent materials

Marlena Gryl, Marcin Koziel, Klaudia Nowakowska, Katarzyna Ostrowska
Jagiellonian University in Kraków, Kraków, Poland; marlena.gryl@uj.edu.pl

External Resource:  Presentation



Poster - 21 Quantum-1595-010_b.pdf

QM/MM-based charge density analysis of protein-ligand complexes: Towards medicinal chemistry and drug design perspective

Saravanan Kandasamy^{1,2,3}

¹Faculty of Chemistry, University of Warsaw, Warsaw, Poland; ²Molecular Biophysics Unit, Indian Institute of Science, Bangalore, India;

³Department of Physics, Periyar University, Salem, India; s.kandasamy@uw.edu.pl

External Resource:  Presentation



Poster - 21 Quantum-1630-011_b.pdf

Experimental and theoretical charge density study of two tetranuclear transition metal clusters with single molecule magnet properties

Sofie Stampe Leiszner¹, **Emil Damgaard-Møller**¹, **Lennard Krause**¹, **Khetpakorn Chakarawet**², **Jeffrey R. Long**³, **Jacob Overgaard**¹

¹Department of Chemistry, Aarhus University, Langelandsgade 140, 8000 Aarhus C, Denmark; ²Department of Chemistry, University of California, Berkeley, Berkeley, California 94720, United States; ³Department of Chemistry and Department of Chemical and Biomolecular Engineering, University of California, Berkeley, Berkeley, California 94720, United States; Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, United States; 201705219@post.au.dk

External Resource:  Presentation



Poster - 21 Quantum-1473-012_b.pdf



Poster - 21 Quantum-1473-012_c.pdf

Understanding the Proton Tautomerism Mechanism in Organic Molecular Ferroelectrics: Insights from Quantum Crystallography

Parthapratim Munshi, Sanjay Dutta, Anil Kumar

Department of Chemistry, School of Natural Science, Shiv Nadar University, Tehsil Dadri, Uttar Pradesh- 201314, India; parthapratim.munshi@snu.edu.in

External Resource:  Presentation



Poster - 21 Quantum-1584-013_b.pdf

Charge Density Studies of *in-situ* Crystallized Liquids with Hirshfeld Atom Refinement, Invariom-Model and Multipole-Model

Michael Peter Patzer

Max-Planck-Institut für Kohlenforschung, Ratingen, Germany; patzer@kofo.mpg.de

External Resource:  Presentation



Poster - 21 Quantum-1725-014_b.pdf

Poster - 22 Ptychography: Ptychography, imaging, coherent scattering

Session Chair: **Sine Larsen**

Session Chair: **Ian Robinson**



4:40pm - 5:40pm

Poster session abstracts

Radomír Kužel



Poster - 22 Ptychography-1949-001.pdf

Ptychographically-assisted X-ray fluorescence nanotomography for characterization of complex materials

Dmitry Karpov¹, **Mirko Holler**², **Dario Ferreira Sanchez**², **Ana Diaz**²

¹European Synchrotron Radiation Facility, 71 Avenue des Martyrs, Grenoble, France; ²Paul Scherrer Institut, Forschungsstrasse 111, Villigen, Switzerland; dmitry.karpov@esrf.fr

External Resource:  Presentation



Poster - 22 Ptychography-1061-002_b.pdf

Coherent X-ray imaging at ID16A: status and plans

Dmitry Karpov¹, Federico Monaco¹, Sylvain Bohic^{1,2}, Murielle Salome¹, Vincent Favre-Nicolin¹, Alexandra Teodora Joita Pacureanu¹, Peter Cloetens¹

¹European Synchrotron Radiation Facility, 71 Avenue des Martyrs, Grenoble, France; ²Inserm UA7 STROBE, Université Grenoble Alpes, 71 Avenue des Martyrs, Grenoble, France; dmitry.karpov@esrf.fr

External Resource:



Poster - 22 Ptychography-1063-003_b.pdf

Toward dynamic ptychography using a spatiotemporal overlap constraint

Gerard Neale Hinsley¹, Grant van Riessen¹, Cameron M Kewish^{1,2}

¹La Trobe University, Melbourne, Australia; ²ANSTO Australian Synchrotron, Clayton, Australia; G.Hinsley@ltnu.edu.au

External Resource:



Poster - 22 Ptychography-1111-004_b.pdf

Coherent X-ray diffraction imaging to investigate structure and morphological evolution of calcium carbonate microparticles

Daniyal Younas¹, Fredrik Kristoffer Mürer¹, Seniz Ucar², Yuriy Chushkin³, Federico Zontone³, Alain Gibaud⁴, Dag Werner Breiby¹, Basab Chattopadhyay¹

¹PoreLab, Department of Physics, Norwegian University of Science and Technology (NTNU), Høgskoleringen 5, 7491 Trondheim, Norway; ²Department of Chemical Engineering, Norwegian University of Science and Technology, Trondheim, Norway; ³ESRF, The European Synchrotron, Grenoble, France; ⁴LUNAM, IMMM, UMR 6283 CNRS, Faculté des Sciences, Le Mans Université, 72085 Le Mans, France; daniyal.younas@ntnu.no

External Resource:



Poster - 22 Ptychography-1112-005_b.pdf

Super-resolution X-ray holography

Jakob Soltau, Malte Vassholz, Markus Osterhoff, Tim Salditt

Georg-August-Universität Göttingen, Göttingen, Germany; jakob.soltau@uni-goettingen.de

External Resource:



Poster - 22 Ptychography-1117-006_b.pdf

Diffraction imaging and tomography investigations on the hydration of gypsum plaster

Michela La Bella^{1,2}, Rogier Besselink², Alexander E. S. Van Driessche², Jonathan P. Wright¹, Carlotta Giacobbe¹, Alejandro Fernandez-Martinez²

¹European Synchrotron Radiation Facility, 71 Avenue Des Martyrs, 38040 Grenoble, France; ²Institut de science de la Terre, Université Grenoble Alpes, 1381 Rue de la Piscine, 38610 Gières, France; michela.la-bella@esrf.fr

External Resource:



Poster - 22 Ptychography-1219-007_b.pdf

Grazing-incidence small angle X-ray photon correlation spectroscopy: limitations and opportunities

Christopher Reiner Greve¹, Meike Kuhn¹, Fabian Eller¹, Michael Andreas Buchhorn¹, Kumar Dinesh², Alexander Hexemer², Guillaume Freychet³, Lutz Wiegart³, Eva M. Herzig¹

¹Herzig Group - Structure Formation & Dynamics, University Bayreuth, Bayreuth, Germany; ²Center for Advanced Mathematics for Energy Research Applications (CAMERA), Lawrence Berkeley National Laboratory, USA; ³National Synchrotron Light Source II, Brookhaven National Laboratory, USA; christopher.greve@uni-bayreuth.de

External Resource:



Poster - 22 Ptychography-920-008_b.pdf

Development and improvement of Bragg coherent diffraction imaging for expanding observable particle-size range

Norihiro Oshime¹, Kenji Ohwada¹, Kento Sugawara¹, Tetsuro Ueno¹, Akihiko Machida¹, Kenji Ishii¹, Hidenori Toyokawa^{1,2}, Yoshihiro Kuroiwa³

¹Synchrotron Radiation Research Center, Kansai Photon Science Institute, Quantum Beam Science Research Directorate, National Institutes for Quantum and Radiological Science and Technology (QST), SPring-8, 1-1-1 Kouto, Sayo, Hyogo 679-5148, Japan; ²Japan Synchrotron Radiation Research Institute, Kouto 1-1-1, Sayo-cho, Sayo-gun, Hyogo 679-5198, Japan; ³Graduate School of Advanced Science and Engineering, Hiroshima University, Higashihiroshima, Hiroshima, 739-8526, Japan; oshime.norihiro@gst.go.jp

External Resource:  Presentation



Poster - 22 Ptychography-1466-009_b.pdf

Wavefield Characterisation of MHz XFEL Pulses

Trey Wilson Guest^{1,2}, Brian Abbey¹, Adrian Mancuso^{1,2}, David Paganin³, Richard Bean², Grant van Riessen¹

¹La Trobe Institute for Molecular Sciences, La Trobe University, Victoria 3086, Australia.; ²European XFEL GmbH, Albert-Einstein-Ring 19, 22761 Hamburg, Germany; ³School of Physics, Monash University, Victoria 3800, Australia; twquest@students.latrobe.edu.au

External Resource:  Presentation



Poster - 22 Ptychography-1468-010_b.pdf

Ptychographic image reconstruction using total variation regularization

Ricarda Nebeling, Iacopo Mochi, Hyun-su Kim, Atoosa Dejkameh, Tao Shen, Manuel Guizar-Sicairos, Yasin Ekinici
Paul Scherrer Institut, Villigen PSI, Switzerland; ricarda.nebeling@psi.ch

External Resource:  Presentation



Poster - 22 Ptychography-1511-011_b.pdf

6:30pm - 7:15pm

Refreshment: Refreshment

Location: **Exhibition and poster area**



7:15pm - 8:45pm

Cultural programme: Concert - Dvorak ensemble

Ensemble Website

Video



Date: Wednesday, 18/Aug/2021

9:00am - 9:50am

KN-16: MicroED: conception, practice and future opportunities

Location: **Terrace 2A**

Session Chair: **Louisa Meshi**

Tamir Gonen



MicroED: conception, practice and future opportunities

Tamir Gonen

HHMI/UCLA, Los Angeles, United States of America; tgonen@g.ucla.edu

External Resource:  Presentation



KN-16-1414-001_b.pdf

9:00am - 9:50am

KN-17: In-situ and In-operando diffraction Studies of Li Ion Battery Electrodes

Location: **Terrace 2B**

Session Chair: **Radovan Cerny**

Gwenaëlle Rousse



In-situ and In-operando diffraction Studies of Li Ion Battery Electrodes

Gwenaëlle ROUSSE

Sorbonne Université - Collège de France, PARIS cedex 5, France; gwenaëlle.rousse@sorbonne-universite.fr

External Resource:  Presentation



KN-17-1420-001_b.pdf

9:00am - 9:50am

KN-18: Electron density, and its interplay with the energy and properties of molecules and solids

Location: **Club A**

Session Chair: **Catharine Esterhuysen**

Julia Contreras-Garcia

Electron density, and its interplay with the energy and properties of molecules and solids

Julia Contreras-Garcia

Sorbonne Université-CNRS, Paris, France; julia.contreras.garcia@gmail.com

External Resource:  Presentation



KN-18-1605-001_b.pdf

9:50am - 10:20am

Morning break 4: Exhibition, posters, coffee/teaLocation: **Exhibition and poster area****MS-41: Macromolecular machines and hybrid methods to crystallography**Location: **Club B**Session Chair: **Michael Landsberg**Session Chair: **Dmitry Svergun**Invited: **Kristina Djinovic-Carugo (Austria), Tanmay Bharat (India)****Introduction**

10:20am - 10:25am

Introduction to session**Michael Landsberg, Dmitry Svergun**

10:20am - 12:45pm



MS-41-1772-001.pdf

10:25am - 10:55am

Structural biology of prokaryotic cell surfaces**Tanmay Bharat**University of Oxford, Oxford, United Kingdom; tanmay.bharat@path.ox.ac.uk

External Resource:



MS-41-1887-002_b.pdf

10:55am - 11:25am

Order from disorder in the sarcomere: FATZ forms a fuzzy complex and phase-separated macromolecular condensates with α -actinin**Kristina DJINOVIC CARUGO**

University of Vienna, Vienna, Austria

External Resource:



MS-41-1575-003_b.pdf

11:25am - 11:45am

Deciphering the role of unique bacterial transcription-associated factor HeID.**Tomáš Koval¹**, Tomáš Kouba², Petra Sudzinová³, Jiří Pospíšil³, Barbora Brezovská³, Jarmila Hnilicová³, Hana Šanderová³, Martina Janoušková³, Michaela Šiková³, Petr Halada³, Michal Sýkora⁴, Ivan Barvík⁵, Jiří Nováček⁶, Mária Trundová¹, Jarmila Dušková¹, Tereza Skálová¹, URee Chon⁷, Katsuhiko S. Murakami⁷, Libor Krásný³, Jan Dohnálek¹¹Institute of Biotechnology of the Czech Academy of Sciences, Vestec, Czech Republic; ²EMBL Grenoble, Grenoble, France; ³Institute of Microbiology of the Czech Academy of Sciences, Prague, Czech Republic; ⁴Institute of Molecular Genetics of the Czech Academy of Sciences, Prague, Czech Republic; ⁵Faculty of Mathematics and Physics, Institute of Physics, Charles University, Prague, Czech Republic; ⁶CEITEC, Masaryk University, Brno, Czech Republic; ⁷The Center for RNA Molecular Biology, Pennsylvania State University, University Park, PA, USA

External Resource:



MS-41-1299-004_b.pdf

11:45am - 12:05pm

Anomalous small-angle X-ray scattering on biological macromolecules at the P12 beamline of EMBL-Hamburg**Andrey Gruzinov¹**, Martin Schroer¹, Clement Blanchet¹, Karen Manalastas-Cantos¹, Alexey Kikhney¹, Nelly Hajizadeh¹, Florian Wieland², Florian Schulz³, Daniel Franke¹, Cy Jeffries¹, Dmitri Svergun¹¹EMBL Hamburg c/o DESY, Notkestrasse 85, 22607 Hamburg, Germany; ²Helmholtz-Zentrum Geesthacht (Außenstelle DESY), Notkestrasse 85, 22607 Hamburg, Germany; ³University of Hamburg, Grindelallee 117, 20146 Hamburg, Germany

External Resource:



MS-41-1606-005_b.pdf

12:05pm - 12:25pm

An asymmetric structure of the filament is key to inducing flagellar curvature and enabling motility in the *Leptospira* spirochete**Fabiana San Martin¹**, Kimberley H Gibson², Felipe Trajtenberg¹, Megan R Brady², Elsie A Wunder³, Mathieu Picardeau⁴, Ariel Mechaly¹, Albert I Ko³, Charles V Sindelar², **Alejandro Buschiazio¹**

¹Lab of Molecular & Structural Microbiology, Institut Pasteur de Montevideo, Mataojo 2020, Montevideo, Uruguay; ²Dept of Molecular Biophysics and Biochemistry, Yale School of Medicine, New Haven, USA; ³Dept of Epidemiology of Microbial Diseases, Yale School of Public Health, New Haven, USA; ⁴Biology of Spirochetes Unit, Institut Pasteur, Paris, France

External Resource:



MS-41-376-006_b.pdf

12:25pm - 12:45pm

Structure of the 80S ribosome from *Candida albicans* revealed by integrative structural biology approach

Yuri Zgadzay^{1,2}, Olga Kolosova², Artem Stetsenko³, Konstantin Usachev¹, Shamil Validov¹, Andrey Rogachev⁴, Albert Guskov^{3,4}, Marat Yusupov^{1,2}

¹Laboratory of Structural Biology, Institute of Fundamental Medicine and Biology, Kazan Federal University, Kazan, Russia;

²Department of Integrated Structural Biology, Institute of Genetics and Molecular and Cellular Biology, University of Strasbourg, Illkirch, France; ³Groningen Biomolecular Sciences and Biotechnology Institute (GBB), University of Groningen, Groningen, the Netherlands;

⁴Moscow Institute of Physics and Technology, Dolgoprudny, Russia

External Resource:



MS-41-1074-007_b.pdf

10:20am - 12:45pm

MS-42: Novel techniques and insights into in vitro and in situ crystallisation for X-ray and electron diffraction.

Location: **Club A**

Session Chair: **Lars Redecke**

Session Chair: **Fasseli Coulibaly**

Invited: **Haruki Hasegawa (USA)**, **Alexandra Ros (USA)**

Introduction

10:20am - 10:25am

Introduction to session

Lars Redecke, Fasseli Coulibaly



MS-42-1773-001.pdf

10:25am - 10:55am

Concurrent crystallization of multiple proteins in a single cell without interfering each other's phase separation events

Haruki Hasegawa

Amgen Inc, South San Francisco, United States of America

External Resource:



MS-42-380-002_b.pdf

10:55am - 11:25am

Microfluidic Tools Reducing Sample Amount in Serial Crystallography with XFELs

Alexandra Ros

Arizona State University, Tempe, United States of America

External Resource:



MS-42-1078-003_b.pdf

11:25am - 11:45am

MyD88 TIR domain higher-order assembly interactions revealed by microcrystal electron diffraction and serial femtosecond crystallography

Max T. B. Clabbers^{2,4}, Susannah Holmes¹, Timothy W. Muusse³, Parimala Vajjhala³, Sara J. Thygesen³, Alpeshkumar K. Malde⁵, Dominic J. B. Hunter^{3,6,7}, Tristan I. Croll⁸, Leonie Flueckiger¹, Jeffrey D. Nanson³, Md. Habibur Rahaman³, Andrew Aquila⁹, Mark S. Hunter⁹, Mengning Liang⁹, Chun Hong Yoon⁹, Jingjing Zhao², Nadia A. Zatsepin¹, Brian Abbey¹, Emma Sieracki⁸, Yann Gambin⁶, Katryn J. Stacey³, Connie Darmanin¹, Bostjan Kobe^{3,7,10}, Hongyi Xu², Thomas Ve⁵

¹Australian Research Council Centre of Excellence in Advanced Molecular Imaging, Department of Chemistry and Physics, La Trobe

Institute for Molecular Science, La Trobe University, Melbourne, Victoria, Australia; ²Department of Materials and Environmental

Chemistry, Stockholm University, Stockholm, Sweden; ³School of Chemistry and Molecular Biosciences, The University of

Queensland, Brisbane, Queensland, Australia; ⁴Department of Biological Chemistry, University of California Los Angeles, Los Angeles,

California, USA; ⁵Institute for Glycomics, Griffith University, Southport, Queensland, Australia; ⁶EMBL Australia Node in Single

Molecule Science, University of New South Wales, Kensington, New South Wales, Australia; ⁷Institute for Molecular Bioscience, The

University of Queensland, Brisbane, Queensland, Australia; ⁸Cambridge Institute for Medical Research, University of Cambridge,

Cambridge, UK; ⁹Linac Coherent Light Source, SLAC National Accelerator Laboratory, Menlo Park, California, USA; ¹⁰Australian

Infectious Diseases Research Centre, The University of Queensland, Brisbane, Queensland, Australia.

External Resource:





MS-42-972-004_b.pdf

11:45am - 12:05pm

The crystallomics pipeline, a shotgun approach on native proteomes to (re)discover the unsuspected

Sylvain Engilberge^{1,2}, Olivier Lemaire³, Marie-Caroline Mueller³, Filip Leonarski³, Chia-Ying Huang¹, Takashi Tomizaki¹, Naohiro Matsugaki⁵, Antoine Royant⁴, Vincent Olieric¹, Meitian Wang¹, Tristan Wagner³

¹Swiss Light Source, Paul Scherrer Institut, Forschungsstrasse 111, Villigen-PSI, 5232, Switzerland; ²European Synchrotron Radiation Facility, 38043 Grenoble, France; ³Max-Planck-Institut für Marine Mikrobiologie, Celsiusstraße 1, 28359, Bremen, Germany;

⁴Structural Biology Research Center, Photon Factory, Institute of Materials Structure Science, High Energy Accelerator Research Organization, Tsukuba, 305-0801, Japan.; ⁵Institut de Biologie Structurale (IBS), Université Grenoble Alpes, CEA, CNRS, 71 avenue des Martyrs, Grenoble Cedex 9, 38044, France

External Resource:



MS-42-1101-005_b.pdf

12:05pm - 12:25pm

Protein crystallization assisted by the crystallophore.

Eric Girard¹, Zaynab Alsaman¹, Adeline Robin¹, Sylvain Engilberge¹, Amandine Roux², François Riobé², Olivier Maury²

¹Institut de Biologie Structurale, Grenoble, France; ²Ecole Normale Supérieure, Lyon, France

External Resource:



MS-42-1020-006_b.pdf

12:25pm - 12:45pm

Protein crystallisation in agarose gel, a cheap and versatile technique

Jose A. Gavira¹, Fiora Artusio², Albert Castellvi³, Roberto Pisano²

¹CSIC, Granada, Spain; ²Politecnico di Torino, Torino, Italy; ³Structural Biology, Molecular Biology Institute of Barcelona, Barcelona, Spain

External Resource:



MS-42-900-007_b.pdf

MS-43: Solid state reactions and dynamics

Location: **Terrace 2B**

Session Chair: **Franziska Emmerling**

Session Chair: **Javier Marti-Rujas**

Invited: **Hiroyoshi Ohtsu (Japan), Paolo Pio Mazzeo (Italy)**

Introduction

10:20am - 10:25am

Introduction to session

Franziska Emmerling, Javier Marti-Rujas



MS-43-1774-001.pdf

10:25am - 10:55am

Stepwise evolution of molecular nanoaggregates inside the pores of a highly flexible Metal-Organic Framework.

Paolo Pio Mazzeo^{1,2}, Davide Balestri¹, Claudia Carraro¹, Nicola Demitri³, Paolo Pelagatti^{1,4}, Alessia Bacchi^{1,2}

¹Dipartimento di Scienze Chimiche, della Vita e della Sostenibilità Ambientale, Università di Parma, Viale delle Scienze, 17A, 43124 Parma (Italy); ²Biopharmanet-TEC, Università degli studi di Parma via Parco Area delle Scienze 27/A, 43124 Parma (Italy); ³Elettra—Sincrotrone Trieste S.S. 14 Km 163.5 in Area Science Park, 34149 Basovizza—Trieste (Italy); ⁴Centro Interuniversitario di Reattività Chimica e Catalisi (CIRCC) Via Celso Ulpiani 27, 70126 Bari (Italy); paolopio.mazzeo@unipr.it

External Resource:



MS-43-494-002_b.pdf

10:55am - 11:25am

Kinetic assembly of coordination networks creates flexible and functional materials

Hiroyoshi Ohtsu

Tokyo Institute of Technology, Meguro-ku, Tokyo, Japan; ohtsu@chem.titech.ac.jp

External Resource:



10:20am - 12:45pm



MS-43-1247-003_b.pdf

11:25am - 11:45am

***In-situ* XRD and PDF investigation of battery fluoride materials $\text{MF}_3 \cdot 3\text{H}_2\text{O}$ (M = Fe, Cr) in controlled atmosphere: accessing new phases with controlled chemistry**

Martin Schreyer¹, Gwilherm Nénert¹, Kerstin Forsberg², Claire V. Colin³

¹Malvern Panalytical B.V., Almelo, Netherlands, The; ²School of Chemical Science and Engineering, Royal Institute of Technology, Teknikringen 42, SE 100 44 Stockholm, Sweden; ³Université Grenoble Alpes, Institut Néel, F-38042 Grenoble, France; martin.schreyer@panalytical.com

External Resource:



MS-43-933-004_b.pdf

11:45am - 12:05pm

Light- and temperature-induced linkage isomerism in a series of Ni^{II} , Cu^{II} and Co^{III} complexes in the solid state

Sylwia Ewa Kutniewska¹, Patryk Borowski¹, Krystyna Deresz¹, Radosław Kaminski¹, Adam Krowczyński¹, Włodzimierz Buchowicz², Dominik Schaniel³, Katarzyna Jarzemska¹

¹Department of Chemistry, University of Warsaw, Żwirki i Wigury 101, 02-089 Warsaw, Poland; ²Department of Chemistry, Warsaw University of Technology, Noakowskiego 3, 00-664 Warsaw, Poland; ³CRM2, Jean Barriol Institute, CNRS UMR 7036, University of Lorraine, BP 70239, Boulevard des Aiguillettes, 54506 Vandœuvre-lès-Nancy, France; skutyla@chem.uw.edu.pl

External Resource:



MS-43-524-005_b.pdf

12:05pm - 12:25pm

Studies of the functional characteristics of adaptive X-ray optical elements based on combination of longitudinal and transverse acoustic waves in wide frequency ranges

Alexander Blagov^{1,2}, Anton Targonskiy^{1,2}, Valentin Akkuratov^{1,2}, Yan Eliovich^{1,2}, Vahan Kocharyan^{3,4}, Anton Kulikov^{1,2}, Artur Movsisyan^{3,4}, Tigran Muradyan³, Yuri Pisarevsky^{1,2}, Alexei Seregin^{1,2}, Mikhail Kovalchuk^{1,2}

¹NRC "Kurchatov institute", 1, Akademika Kurchatova pl., Moscow, Russia, 123182; ²FSRC "Crystallography and photonics" RAS, 59, Leninskii pr., Moscow, Russia, 119333; ³Institute of Applied Problems of Physics NAS of Armenia, 25, Hrachya Nersissian Str., Yerevan, Republic of Armenia, 0014; ⁴Tomsk Polytechnic University, 30, Lenin Avenue, Tomsk, Russia, 634050; Targonskiy_AV@nrcki.ru

External Resource:



MS-43-513-006_b.pdf

12:25pm - 12:45pm

***In situ* control of Photochromic properties with dual photoreactive soft crystal**

Akiko Sekine, Yuta Yamazaki, Masato Tanaka, Hidehiro Uekusa

Department of Chemistry, Tokyo Institute of Technology, Tokyo, Japan; asekine@chem.titech.ac.jp

External Resource:



MS-43-888-007_b.pdf

MS-44: Beyond pure point diffraction: Theory and application of diffuse scattering

Location: Club H

Session Chair: Nicolae Strungaru

Session Chair: Uwe Grimm

Invited: Chrizaldi Neil Manibo (Germany), Ella Mara Schmidt (Germany)

Introduction

10:20am - 10:25am

Introduction to session

Nicolae Strungaru, Uwe Grimm



MS-44-1775-001.pdf

10:25am - 10:55am

The mathematics of absolutely continuous diffraction

Chrizaldi Neil Manibo

Bielefeld University, Bielefeld, Germany; cmanibo@math.uni-bielefeld.de

10:20am - 12:45pm

External Resource:



MS-44-276-002_b.pdf

10:55am - 11:25am

Mean field theory calculations to model single crystal diffuse scattering

Ella Mara Schmidt, Johnathan Bulled, Andrew Goodwin

University of Oxford, Oxford, United Kingdom; ella.schmidt@chem.ox.ac.uk

External Resource:



MS-44-401-003_b.pdf

11:25am - 11:45am

KOSSEL LINES AND X-RAY LOCALIZED CONICAL MODES

Vladimir Alekseevich Belyakov

Landau Institute for Theoretical Physics, Moscow, Russian Federation; bel@landau.ac.ru

External Resource:



MS-44-617-004_b.pdf

11:45am - 12:05pm

Characterization of the correlated disorder in $\text{Ge}_2\text{Bi}_4\text{Te}_7$

Matthias Quintelier, Stefano Canossa, Mylène Hendrickx, Romy Poppe, Joke Hadermann

University of Antwerp, Wommelgem, Belgium; matthias.quintelier@student.uantwerpen.be

External Resource:



MS-44-1210-005_b.pdf

12:05pm - 12:25pm

Tuning of disordered local structure in Prussian Blue analogues

Yevheniia Kholina, Arkadiy Simonov

ETH Zurich, Zurich, Switzerland; arkadiy.simonov@mat.ethz.ch

External Resource:



MS-44-1272-006_b.pdf

12:25pm - 12:45pm

Implementation for coping with sample and instrument effects for reverse Monte Carlo modelling of total scattering data

Yuanpeng Zhang

Oak Ridge National Laboratory, Knoxville, United States of America; zhangy3@ornl.gov

External Resource:



MS-44-754-007_b.pdf

MS-45: Frustrated magnetic order and emerging science

Location: **Club C**

Session Chair: **Romain Sibille**

Session Chair: **Geetha Balakrishnan**

Invited: **Beauvois Ketty** (France), **Nicolas Gauthier** (USA)

Introduction

10:20am - 10:25am

Introduction to session

Roman Sibille, **Geetha Balakrishnan**



MS-45-1776-001.pdf

10:25am - 10:55am

Dimer physics in the frustrated Cairo pentagonal antiferromagnet $\text{Bi}_2\text{Fe}_4\text{O}_9$

Ketty Beauvois^{1,2}, **Virginie Simonet**³, **Sylvain Petit**⁴, **Julien Robert**³, **Frédéric Bourdarot**², **Marin Gospodinov**⁵, **Sacha Mukhin**⁶, **Rafik Ballou**³, **Vassil Skumryev**⁷, **Eric Ressouche**²

¹Institut Laue Langevin, Grenoble, France; ²CEA, IRIG/DEPHY/MEM-MDN, Grenoble, France; ³Institut Néel, CNRS, Grenoble, France; ⁴CEA-CNRS, LLB Saclay, France; ⁵Institute of Solid State Physics, Bulgarian Academy of Sciences, Bulgaria; ⁶Russian Academy of science, Russia; ⁷Universitat Autònoma de Barcelona, Spain; beauvois@ill.fr

External Resource:



MS-45-209-002_b.pdf

10:55am - 11:25am

Characterizing the local charge density to determine complex magnetic correlations, and vice versa

Nicolas Gauthier

Stanford University & SLAC National Accelerator Laboratory, Stanford, California 94305, USA; nicolas.gauthier@stanford.edu

External Resource:



MS-45-1159-003_b.pdf

11:25am - 11:45am

Magnetic structure and interactions in 2D layered van der Waals semiconductors CrPS₄ and MnPSe₃ probed with neutron scattering

Stuart Calder¹, **Amanda Haglund**², **Yaohua Liu**¹, **Daniel Pajeroski**¹, **Huibo Cao**¹, **Travis Williams**¹, **Alexander Kolesnikov**¹, **Vasile Garlea**¹, **David Mandrus**²

¹Oak Ridge National Laboratory; ²University of Tennessee; caldersa@ornl.gov

External Resource:



MS-45-1104-004_b.pdf

11:45am - 12:05pm

Geometric frustration on the trillium lattice in a magnetic metal-organic framework

Johnathan M. Bulled¹, **Joseph A. M. Paddison**^{2,3}, **Andrew Wildes**⁴, **Elsa Lhotel**⁵, **Breogan Pato-Doldan**⁶, **L. Claudia Gomez-Aguirre**⁷, **Paul J. Saines**⁸, **Andrew L. Goodwin**¹

¹Inorganic Chemistry Laboratory, University of Oxford, South Parks Rd., Oxford OX1 3QR, U.K.; ²Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, U.S.A.; ³Churchill College, University of Cambridge, Storey's Way, Cambridge CB3 0DS, U.K.; ⁴Institut Laue-Langevin, BP156, 71 Avenue des Martyrs, 38000, Grenoble, France; ⁵Institut Néel, 25 Avenue des Martyrs, 38042 Grenoble, France; ⁶Department of Chemistry, University of Bergen, P.O. Box 7803, N-5020 Bergen, Norway; ⁷Department of Fundamental Chemistry and CICA, Faculty of Sciences University of A Coruña, 15071 A Coruña, Spain; ⁸School of Physical Sciences, University of Kent, Canterbury CT2 7NH, U.K.; johnathan.bulled@balliol.ox.ac.uk

External Resource:



MS-45-1301-005_b.pdf

12:05pm - 12:25pm

Investigating Kosterlitz-Thouless physics in the triangular lattice antiferromagnet TmMgGaO₄

Benjamin A. Frandsen¹, **Zhiling Dun**², **Raju Baral**¹, **Martin Mourigal**²

¹Brigham Young University, Provo, United States of America; ²Georgia Institute of Technology, Atlanta, United States of America; benfrandsen@byu.edu

External Resource:



MS-45-895-006_b.pdf

12:25pm - 12:45pm

Nanoscale distortions and ground state selection in geometrically frustrated magnets

Alexandros Lappas¹, **Benjamin Frandsen**², **Emil Bozin**³

¹Foundation for Research and Technology - Hellas, 71110 Heraklion, Crete, Greece; ²Brigham Young University, Provo, Utah 84602, USA; ³Brookhaven National Laboratory, Upton, New York 11973, USA; lappas@iesl.forth.gr

External Resource:



MS-45-850-007_b.pdf

10:20am - 12:45pm

MS-46: In-situ and in operando studies of battery materials

Location: Club D



Session Chair: **Vanessa Kate Peterson**
Session Chair: **Claire Villeveille**
Invited: **Karena Chapman (USA), Sandrine Lyonnard (France)**

Introduction

10:20am - 10:25am

Introduction to session

Vanessa Kate Peterson, Claire Villeveille



MS-46-1777-001.pdf

10:25am - 10:55am

Dynamic heterogeneity in transition metal oxide cathodes

Karena Chapman

Stony Brook University, Stony Brook, United States of America; karena.chapman@stonybrook.edu

External Resource:



MS-46-1126-002_b.pdf

10:55am - 11:25am

Operando characterization of battery anodes using mXRD and combined SAXS/WAXS

Sandrine Lyonnard, Samuel Tardif

CEA IRIG, Grenoble, France; sandrine.lyonnard@cea.fr

External Resource:



MS-46-1412-003_b.pdf

11:25am - 11:45am

Insight into the charging-discharging of magnetite electrodes: In-situ XAS study

Chandrani Nayak, Abharana N. S. N. Jha, Dibyendu Bhattacharyya

Bhabha Atomic Research Centre, Mumbai, India; nayakc@barc.gov.in

External Resource:



MS-46-199-004_b.pdf

11:45am - 12:05pm

Powerful SAS techniques for operando analysis of battery materials

Eneli Härk¹, Ben Kent², Sebastian Risse¹, Rafael Müller¹, Matthias Ballauff³, Yan Lu¹

¹Department for Electrochemical Energy Storage, Helmholtz-Zentrum Berlin, Hahn-Meitner-Platz 1, 14109, Berlin, Germany; ²School of Chemistry, UNSW Sydney NSW 2052, Australia; ³Institut für Chemie und Biochemie Freie Universität Berlin Takustrasse 3, 14195 Berlin, Germany; eneli.haerk@helmholtz-berlin.de

External Resource:



MS-46-630-005_b.pdf

12:05pm - 12:25pm

Redox oscillations in 18650-type lithium-ion cell revealed by in-operando Compton scattering imaging

Kosuke Suzuki¹, Shunta Suzuki¹, Yuji Otsuka¹, Naruki Tsuji², Kirsi Jalkanen³, Jari Koskinen³, Kazushi Hoshi¹, Ari-Pekka Honkanen⁴, Hasnain Hafiz⁵, Yoshiharu Sakurai², Mika Kanninen³, Simo Huotari⁴, Arun Bansil⁶, Hiroshi Sakurai¹, Bernardo Barbiellini^{7,6}

¹Gunma University, Kiryu, Japan; ²Japan Synchrotron Radiation Research Institute, SPring-8, Sayo, Japan; ³Akkurate Oy, Kaarikatu 8b, 20760 Kaarina, Finland; ⁴University of Helsinki, P.O. Box 64, FI-00014 Helsinki, Finland; ⁵Carnegie Mellon University, Pittsburgh, USA; ⁶Northeastern University, Boston, USA; ⁷LUT University, FI-53850 Lappeenranta, Finland; kosuzuki@gunma-u.ac.jp

External Resource:



MS-46-1015-006_b.pdf

12:25pm - 12:45pm

Optimization of in-situ 3D electron diffraction in an electrochemical liquid cell for crystal structure determination of energy materials

Mylene Hendrickx, Joke Hadermann

University of Antwerp, Antwerp, Belgium; mylene.hendrickx@uantwerpen.be

External Resource:





MS-46-1189-007_b.pdf

MS-47a: Nanocrystalline materials I

Location: 223-4

Session Chair: **Cinzia Giannini**

Session Chair: **Jinong Zhu**

Invited: **Junliang Sun** (China), **Ulf Olsson** (Sweden)

Introduction

10:20am - 10:25am

Introduction to session

Cinzia Giannini, **Jinong Zhu**



MS-47a-1778-001.pdf

10:25am - 10:55am

The colloidal structure of a regenerated cellulose fiber

Ulf Olsson¹, **Marta Gubitosi**¹, **Shirin Asadi**^{1,2}, **Herbert Sixta**², **Luigi Gentile**³, **Cinzia Giannini**⁴

¹Lund University, Lund, Sweden; ²Aalto University, Finland; ³University of Bari, Bari, Italy; ⁴Institute of Crystallography, CNR, Bari, Italy; ulf.olsson@fkem1.lu.se

External Resource:



MS-47a-952-002_b.pdf

10:55am - 11:25am

Structure determination of nanocrystals

Junliang Sun

Peking University, Beijing, China, People's Republic of; junliang.sun@pku.edu.cn

External Resource:



MS-47a-1850-003_b.pdf

11:25am - 11:45am

Thermal disorder and mechanical anisotropy in nanocrystals

Alberto Leonardi^{1,2}, **Matteo Leoni**³, **Michael Engel**²

¹ISIS Neutron and Muon Facility, UKRI-Science and Technical Facility Council, Didcot, United Kingdom; ²Institute for Multiscale Simulation, Friedrich-Alexander University Erlangen-Nürnberg; ³Saudi Aramco Research & Development Center; alberto.leonardi@stfc.ac.uk

External Resource:



MS-47a-1153-004_b.pdf

11:45am - 12:05pm

Interplay between size, morphology, microstructure defects and optoelectronic properties of CdSe nanocrystals

Stefan Neumann¹, **Martin Rudolph**¹, **Christina Menter**^{2,3}, **Ahmed Salaheldin Mahmoud**^{2,3}, **Doris Segets**⁴, **David Rafaja**¹

¹Institute of Materials Science, TU Bergakademie Freiberg, Germany; ²Institute of Particle Technology (LFG), Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Germany; ³Interdisciplinary Center for Functional Particle Systems (FPS), Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Germany; ⁴Process Technology for Electrochemical Functional Materials and Center for Nanointegration Duisburg-Essen (CENIDE), University Duisburg-Essen, Germany; St.Neumann@iww.tu-freiberg.de

External Resource:



MS-47a-575-005_b.pdf

12:05pm - 12:25pm

Spinel ferrite nanoparticles in core shell architecture for heat release

Marco Sanna Angotzi¹, **Valentina Mameli**¹, **Claudio Cara**¹, **Anna Musinu**¹, **Claudio Sangregorio**², **Jana Vejpravova**³, **Carla Cannas**¹

¹Department of Chemical and Geological Sciences, University of Cagliari, S.S. 554 bivio per Sestu, 09042 Monserrato (CA), Italy; ²Istituto di Chimica dei Composti OrganoMetallici - Consiglio Nazionale delle Ricerche (ICCOM-CNR), Via Madonna del Piano 10, 50019 Sesto Fiorentino (FI), Italy; ³Department of Condensed Matter Physics, Charles University, Ke Karlovu 5, 12116 Prague 2, Czech Republic; sannamarco91@gmail.com

External Resource:





MS-47a-297-006_b.pdf

12:25pm - 12:45pm

Monodisperse Cesium lead bromide perovskite nanocrystals (NCs) CsPbBr₃ with bright and stable green photoluminescence for application light emitters devices.

Nabila Jarmouni¹, Francesco Pineider², Marco Tomaiuolo², Said Benmokhtar¹

¹Laboratory of Physical Chemistry of Materials, Department of Chemistry, Faculty of Sciences, University Hassan II of Casablanca, Casablanca, Morocco; ²Department of Chemistry and Industrial Chemistry, University of Pisa, Italy; nabilajarmouni@gmail.com

External Resource:



MS-47a-645-007_b.pdf

MS-48: Combination of X-rays and electrons for structure characterization

Location: **Terrace 2A**

Session Chair: **Joke Hadermann**

Session Chair: **Junliang Sun**

Invited: **Stef Smeets (Netherlands), Tatiana Gorelik (Germany)**

Introduction

10:20am - 10:25am

Introduction to session

Joke Hadermann, Junliang Sun



MS-48-1779-001.pdf

10:25am - 10:55am

X-ray powder diffraction and electron single crystal diffraction – two techniques for structure analysis of nanocrystals

Tatiana Gorelik

University of Ulm, Ulm, Germany; tatiana.gorelik@uni-ulm.de

External Resource:



MS-48-1109-002_b.pdf

10:55am - 11:25am

In the age of electrons, do we still need powder diffraction?

Stef Smeets

Netherlands eScience Center, Amsterdam, The Netherlands; s.smeets@esciencecenter.nl

External Resource:



MS-48-1483-003_b.pdf

11:25am - 11:45am

The long-time elusive structure of magadiite, solved by 3D electron diffraction and model building

Yasar Krysiak¹, Marcel Maslyk², Bruna N. N. Silva³, Sergi Plana-Ruiz^{4,5}, Hipassia M. Moura⁶, Erica O. Munsignatti⁶, Viviane S. Vaiss³, Ute Kolb^{2,4}, Wolfgang Tremel², Lukáš Palatinus⁷, Alexandre A. Leitão¹, Bernd Marler⁸, Heloise O. Pastore⁶

¹Inst. Inorg. Chem., University of Hannover, Germany; ²Inst. Inorg. Chem. Analytical Chem., University of Mainz, Germany; ³Group of Phys. Chem. of Solids and Interfaces, Depart. Chem., Universidade Federal de Juiz de Fora, Brazil; ⁴Depart. Mater. Geoscience, University of Darmstadt, Germany; ⁵LENS, MIND/IN2UB, Engineer Depart.: Electronics section, Universitat de Barcelona, Catalonia; ⁶Micro Mesoporous Molecular Sieves Group, Inst. Chem., University of Campinas, Brazil; ⁷Departm. Structure Analysis, Inst. Physics, Czech Academy of Sciences, Czech Republic; ⁸Inst. Geol. Mineral., Geophysics, Ruhr University Bochum, Germany; vasar.krysiak@aca.uni-hannover.de

External Resource:



MS-48-941-004_b.pdf

11:45am - 12:05pm

Structure and stability of δ-indomethacin

Iryna Andrusenko¹, Enrico Mugnaioli¹, Mauro Gemmi¹, Arianna E. Lanza^{1,2}, Victoria Hamilton³, Charlie L. Hall³, Jason Potticary³, Simon R. Hall³, Anna M. Piras⁴, Ylenia Zambito⁴

¹Istituto Italiano di Tecnologia, Pisa, Italy; ²ELDICO Scientific AG, Villigen, Switzerland; ³School of Chemistry, University of Bristol, Bristol, UK; ⁴Department of Pharmacy, University of Pisa, Pisa, Italy; iryna.andrusenko@iit.it

External Resource:



10:20am - 12:45pm



MS-48-966-005_b.pdf

12:05pm - 12:25pm

A Novel High-Pressure Tin Oxynitride $\text{Sn}_2\text{N}_2\text{O}$

Philipp Gollé-Leidreiter^{1,4}, Leonore Wiehl¹, Shrikant Bhat², Ute Kolb^{1,3}, Ralf Riedel¹

¹FB Material- und Geowissenschaften, Technische Universität Darmstadt, Alarich Weiss Straße 2, 64287 Darmstadt, Germany;

²Photon Science, DESY, Notkestrasse 85, 22607 Hamburg, Germany; ³Institut für Physikalische Chemie, Johannes Gutenberg-

Universität Mainz, Saarstraße 10-14, 55128 Mainz, Germany; ⁴Fraunhofer ISC Neunerplatz 2, 97082 Würzburg, Germany;

philipp.golle-leidreiter@isc.fraunhofer.de

External Resource:



MS-48-1263-006_b.pdf

12:25pm - 12:45pm

Low Dose Electron Diffraction Tomography (LD-EDT) in TEM: Application on an hydrated Al arsenate mineral

Emre Yörük, Holger Klein, Stephanie Kodjikian

Université Grenoble Alpes and CNRS, Institut Néel, 38000, Grenoble, France; emre.yoruk@neel.cnrs.fr

External Resource:



MS-48-646-007_b.pdf

SF-3: Software Fayre 3

Location: **221-2**

Session Chair: **Martin Lutz**

Session Chair: **Claudia Millán**

<http://www.cryst.chem.uu.nl/lutz/>

10:20am - 11:05am

Olex2

Horst Puschmann

OlexSys / Durham University, Durham, United Kingdom; horst.puschmann@gmail.com

External Resource:



11:05am - 11:50am

NoSpherA2: non-spherical form factors in Olex2

Florian Kleemiss

University of Regensburg, Regensburg, Germany; florian.kleemiss@ur.de

External Resource:



IamaGOET - an interface for quantum crystallography

Lorraine Andrade Malaspina

University of Bern, Bern, Switzerland; lorraine.malaspina@gmail.com

External Resource:



10:20am - 12:45pm

12:45pm - 2:45pm

Lunch 4: Exhibition, posters, lunches

Location: **Exhibition and poster area**

Meeting ECA2: ECA Council Meeting

Location: **Club H**

Session Chair: **Udo Heinemann**

Session Chair: **Arie van der Lee**

ECA council meeting 2

12:45pm - 2:45pm

Workshop - Journals: Journal Author Workshop. From data to publication

Location: **Club A**

Session Chair: **Andrew Allen**

Session Chair: **Michele Zema**

Panelists: Elspeth Garman (Acta D); Chiara Massera (Acta E); Andrew Allen (Editor-in-Chief)

Managing editors and IUCr staff: Louise Jones (Acta D); Michele Zema (Executive Outreach Officer)

Videos: **E. Garman - C. Massera - A. Allen - L. Jones**

1:00pm - 2:00pm

MS-49: Protein design and engineering

Location: **Club A**

Session Chair: **Charlotte Uetrecht**

Session Chair: **Sheena McGowan**

Invited: **Elizabeth M.J. Gillam (Australia)**, **Mauri Kostianinen (Finland)**

Introduction

2:45pm - 5:10pm

2:45pm - 2:50pm



MS-49-1780-001.pdf

2:50pm - 3:20pm

Using Ancestral Sequence Reconstruction to Create Robust, Highly Expressed Proteins for Crystallography

Elizabeth M.J. Gillam¹, Raine E.S. Thomson¹, Stephlina A. D'Cunha¹, Kurt L. Harris¹, Gabriel Foley¹, Mikael Boden¹, Aaron G. Bart², Emily E. Scott²

¹The University of Queensland, Brisbane, Australia; ²University of Michigan, Ann Arbor, MI, United States

External Resource: Presentation



MS-49-1422-002_b.pdf

3:20pm - 3:50pm

Protein cage directed nanoparticle superlattices

Mauri Kostiainen

Aalto University, Espoo, Finland

External Resource: Presentation



MS-49-251-003_b.pdf

3:50pm - 4:10pm

The bright-side and the dark-side of computational protein stabilization

Martin Marek^{1,2}, Klara Markova¹, Antonin Kunka^{1,2}, Klaudia Chmelova¹, Martin Havlasek¹, Petra Babkova^{1,2}, Sérgio Marques^{1,2}, Michal Vasina^{1,2}, Joan Iglesias-Planas¹, Radka Chaloupkova^{1,2}, David Bednar^{1,2}, Zbynek Prokop^{1,2}, Jiri Damborsky^{1,2}

¹Masaryk University, Brno, Czech Republic; ²International Clinical Research Center, St. Anne's University Hospital Brno, Czech Republic

External Resource: Presentation



MS-49-166-004_b.pdf

4:10pm - 4:30pm

Enzyme engineering by random mutagenesis: structural and functional studies of modified plant-type L-asparaginase (EcAll)

Joanna Loch¹, Agnieszka Klonecka¹, Kinga Kądziołka¹, Piotr Bonarek², Jakub Barciszewski³, Krzysztof Lewiński¹, Mariusz Jaskolski^{3,4}

¹Jagiellonian University, Faculty of Chemistry, Krakow, Poland; ²Jagiellonian University, Faculty of Biochemistry, Biophysics and Biotechnology, Krakow, Poland; ³Institute of Bioorganic Chemistry, Polish Academy of Sciences, Poznan, Poland; ⁴Faculty of Chemistry, A. Mickiewicz University, Poznan, Poland

External Resource: Presentation



MS-49-835-005_b.pdf

4:30pm - 4:50pm

Computational design of symmetric eight and nine-bladed β -propellers

Bram Mylemans, Arnout RD Voet

KU Leuven, Heverlee, Belgium

External Resource: Presentation



MS-49-1092-006_b.pdf

4:50pm - 5:10pm

Structural evidence for the bleaching caused by oxygen in rsCherry

Thi Yen Hang Bui¹, Benjamin Moeyaert¹, Ludovic Pecqueur², Bindu Srinivasu³, Anastassios Economou³, Marc Fontecave², Peter Dedecker¹, Luc Van Meervelt¹

¹Biochemistry, Molecular and Structural Biology; Department of Chemistry, KU Leuven, Belgium; ²Chemistry of Biological Processes, Collège de France, Paris, France; ³Laboratory of Molecular Bacteriology, Rega Institute, KU Leuven, Belgium; yenhang.bui@gmail.com

External Resource: Presentation



MS-49-215-007_b.pdf

2:45pm - 5:10pm

MS-51: Molecular magnets and metal-organic frameworks including quantum crystallography approaches

Location: **Club B**

Session Chair: **Jozef Kozisek**

Session Chair: **Verónica Paredes-García**

Invited: **Ivan Němec (Czech Republic), Lorraine Andrade Malaspina (France)**

Introduction

2:45pm - 2:50pm

Introduction to session

Jozef Kožíšek, Veronica Paredes-Garcia



MS-51-1781-001.pdf

2:50pm - 3:20pm

Semicoordination in Co(II) Single-Ion Magnets

Ivan Nemecek^{1,2}, Ondrej Frantisek Fellner¹, Lubomír Havlíček², Radovan Herchel¹

¹Palacky University, Olomouc, Czech Republic; ²Ceitec Brno University of Technology, Czech Republic; ivan.nemec@upol.cz

External Resource:



MS-51-961-002_b.pdf

3:20pm - 3:50pm

Quantum crystallography of systems with agostic interactions

Lorraine Andrade Malaspina, Simon Grabowsky

University of Bern, Department of Chemistry, Biochemistry and Pharmaceutical Sciences, Switzerland; lorraine.malaspina@gmail.com

External Resource:



MS-51-909-003_b.pdf

3:50pm - 4:10pm

Field-dependent magnetic anisotropy in a single-ion magnet measured using polarized neutron powder diffraction

Emil Andreasen Klahn¹, Andreas Munch Thiel¹, Iurii Kibalin², Arsen Gukasov², Jacob Overgaard¹

¹Dept. of Chemistry, Aarhus University, Langelandsgade 140, 8000 Aarhus C, Denmark; ²Laboratoire Léon Brillouin, CEA-CNRS, CE-Saclay, 91191 Gif-sur-Yvette, France; eklahn@chem.au.dk

External Resource:



MS-51-1091-004_b.pdf

4:10pm - 4:30pm

Through-space intervalence charge transfer in cobalt based Metal-organic framework: an experimental and theoretical study

AKASHDEEP NATH, SURYAKANTA TANTY, VENNAPUSA SIVARANJANA REDDY, SUKHENDU MANDAL

IISER THIRUVANANTHAPURAM, KERALA, INDIA; iakashdeepnath16@iisertvm.ac.in

External Resource:



MS-51-528-005_b.pdf

4:30pm - 4:50pm

Magnetism of 2D Thiocyanates

Matthew James Cliffe¹, Madeleine Geers^{1,2}, Laura Cañadillas Delgado², Euan Bassey³

¹School of Chemistry, University of Nottingham, University Park, United Kingdom; ²Institut Laue Langevin, Grenoble, France; ³Dept. of Chemistry, Lensfield Road, University of Cambridge; matthew.cliffe@nottingham.ac.uk

External Resource:



MS-51-796-006_b.pdf

4:50pm - 5:10pm

High-Pressure Studies of Single-Molecule Magnets

Andreas Munch Thiel, Marie Steenberg Norre, Jacob Overgaard

Dept. of Chemistry, Aarhus University, Langelandsgade 140, 8000 Aarhus C, Denmark; andreasmt@chem.au.dk

External Resource:



MS-51-1271-007_b.pdf

MS-52: Combining X-ray diffraction and spectroscopy to characterise materials

Location: **Terrace 2A**

Session Chair: **Carlo Meneghini**

Session Chair: **Siegbert Schmid**

Invited: **Ilaria Carlomagno** (Italy), **Marco Giorgetti** (Italy)

Introduction

2:45pm - 2:50pm

Introduction to session

Carlo Meneghini, **Siegbert Schmid**



MS-52-1782-001.pdf

2:50pm - 3:20pm

Structure and charge monitoring of battery materials: long range vs. short range in Prussian Blue Analogous

Marco Giorgetti

University of Bologna, Bologna, Italy; marco.giorgetti@unibo.it

External Resource:



MS-52-759-002_b.pdf

3:20pm - 3:50pm

Diffraction and Spectroscopy: characterising thin ferromagnetic films from the local scale to the long-range... and beyond

Ilaria Carlomagno¹, **Jakub Drnec**², **Roberto Felici**³, **Carlo Meneghini**⁴

¹Elettra Sincrotrone Trieste, Basovizza, Italy; ²ESRF, Grenoble, France; ³SPIN-CNR, Rome, Italy; ⁴Università Roma Tre, Rome, Italy; ilaria.carlomagno@elettra.eu

External Resource:



MS-52-691-003_b.pdf

3:50pm - 4:10pm

Combining X-ray absorption and diffraction to relate structure to the activity in catalysts for CO₂ valorization reactions

Paula Macarena Abdala, **Muhammad Awais Naeem**, **Sung Min Kim**, **Athanasia Tsoukalou**, **Alexey Fedorov**, **Christoph Müller**
ETH Zurich, Zürich, Switzerland; abdalap@ethz.ch

External Resource:



MS-52-1137-004_b.pdf

4:10pm - 4:30pm

XAS, IR and XRD analysis for structural characterization of rare minerals: new occurrence of demantoid garnets in Sa Spinabedda mine (Sardinia – Italy)

Nicola Precisvalle¹, **Annalisa Martucci**¹, **Costanza Bonadiman**¹, **Simone Pollastri**², **Chiaramaria Stani**²

¹Physics and Earth Sciences Department, University of Ferrara, Via Saragat 1, 44122 Ferrara, Italy; ²Elettra - Sincrotrone Trieste, ss 14, km 163.5, 34149 Basovizza, Trieste Italy.; prcncl@unife.it

External Resource:



MS-52-757-005_b.pdf

4:30pm - 4:50pm

Effects of Li⁺ addition rate during the synthesis of LiFePO₄: Combining X-ray diffraction and spectroscopy techniques to determine average and local structure.

Michelle Thiebaut^{1,2,3}, **Caren Billing**¹, **David Billing**^{1,3}, **Deena Naidoo**^{1,3}

¹University of the Witwatersrand, Johannesburg, South Africa; ²National Research Foundation, South Africa; ³Centre of Excellence in Strong Materials (DSI - NRF CoE-SM); 736407@students.wits.ac.za

External Resource:



MS-52-316-006_b.pdf

4:50pm - 5:10pm

Ultraviolet-assisted synthesis and structural characterization of the Pd nanoparticles on the CeO₂ substrate

Mikhail Viktorovich Kirichkov, Vladimir Andreevich Polyakov, Andrei Alexandrovich Tereshchenko, Victor Vasilievich Shapovalov, Alexander Alexandrovich Guda, Alexander Vladimirovich Soldatov

The Smart Materials Research Institute, Rostov-on-Don, Russian Federation; mikhail.kirichkov@gmail.com

External Resource:



MS-52-469-007_b.pdf

2:45pm - 5:10pm

MS-53: Function and application of porous crystals

Location: **Club C**

Session Chair: **Karena Chapman**

Session Chair: **Fernando Uribe-Romo**

Introduction

2:45pm - 2:50pm

Introduction to session

Karena Chapman, **Fernando Uribe-Romo**



MS-53-1784-001.pdf

2:50pm - 3:20pm

Densely Packed UV-Visible Light Responsive Photocatalytic Pairs in Hexagonally Arrayed Silicate Nanochannels for Hydrogen Production

Je-Wei Chang^{1,2}, An-Chung Su², Ying-Huang Lai³, U-Ser Jeng^{1,2}

¹National Synchrotron Radiation Research Center (NSRRC), Hsinchu, Taiwan; ²National Tsing Hua University Department of Chemical Engineering; ³Tungshai University Department of Chemistry; weinanochang@gmail.com

External Resource:



MS-53-1281-002_b.pdf

3:20pm - 3:50pm

MOFs as hosts to analogues of complex magnetic phases

Emma H Wolpert¹, François-Xavier Coudert², Andrew L Goodwin³

¹Imperial College London, United Kingdom; ²Université Paris Sciences et Lettres, France; ³University of Oxford, Oxford, United Kingdom; e.wolpert@imperial.ac.uk

External Resource:



MS-53-585-003_b.pdf

3:50pm - 4:15pm

NMR crystallography of 2D and 3D assemblies of functional molecules

Martin Dracinsky, Guillaume Bastien, Carina Santos-Hurtado, Jiri Kaleta

Institute of Organic Chemistry and Biochemistry AS CR, Prague, Czech Republic; dracinsky@uochb.cas.cz

External Resource:



MS-53-980-004_b.pdf

4:15pm - 4:40pm

From CO₂ to dimethyl ether: mesostructured acidic oxides for methanol dehydration to design bifunctional catalysts

Fausto Secci¹, Claudio Cara¹, Elisabetta Rombi¹, Marco Sanna Angotzi¹, Sarah Lai², Kai Skrodzky³, Nicola Pinna³, Mauro Mureddu², Carla Cannas¹

¹University of Cagliari, Monserrato (CA), Italy; ²Sotacarbo SpA, Carbonia (SU), Italy; ³Humboldt University, Berlin, Germany; fausto.secci@unica.it

External Resource:





MS-53-1073-005_b.pdf

MS-54: Materials for energy conversion and storage



Location: **Terrace 2B**

Session Chair: **Jean-Marc Joubert**

Session Chair: **Stefan Adams**

Invited: **Yaroslav Filinchuk** (Belgium), **Kent Griffith** (USA)

Introduction

2:45pm - 2:50pm



Introduction to session

Jean-Marc Joubert, **Stefan Adams**



MS-54-1785-001.pdf

2:50pm - 3:20pm



Accessing micro- and macroscopic pictures of gas adsorption by in situ powder diffraction

Yaroslav Filinchuk¹, **Xiao Li**¹, **Iurii Dovgaliuk**², **Dmitry Chernyshov**³

¹UCLouvain, Louvain-la-Neuve, Belgium; ²École normale supérieure, Paris, France; ³SNBL/ESRF, Grenoble, France;
yaroslav.filinchuk@uclouvain.be

External Resource:



MS-54-1096-002_b.pdf

3:20pm - 3:50pm



Parallel and serial reduction pathways in complex oxide lithium-ion battery anodes

Kent J. Griffith, **Kenneth R. Poeppelmeier**

Northwestern University, Evanston, United States of America; kent.griffith@northwestern.edu

External Resource:



MS-54-804-003_b.pdf

3:50pm - 4:10pm



Metal hydroborates as solid-state electrolytes

Radovan Cerny

University of Geneva, Geneva, Switzerland; Radovan.Cerny@unige.ch

External Resource:



MS-54-699-004_b.pdf

4:10pm - 4:30pm



Atomistic modelling as a complementary tool for diffraction studies

Max Avdeev

Australian Nuclear Science and Technology Organisation, Lucas Heights, Australia; max@ansto.gov.au

External Resource:



MS-54-779-005_b.pdf

4:30pm - 4:50pm



Degradation mechanisms and thermal stability of vacancy-free Na₂Fe[Fe(CN)₆]: The impact of water and guest cations

Dickson Ojwang, **Hanna Bostroem**, **William Robert Brant**

Uppsala University, Uppsala, Sweden; william.brant@kemi.uu.se

External Resource:



MS-54-570-006_b.pdf

4:50pm - 5:10pm



Structure-properties correlations unlocked through exquisitely sensitive powder diffraction

Peter Khalifah^{1,2}

¹Stony Brook University; ²Brookhaven National Laboratory; kpete@bnl.gov

External Resource:



MS-54-1083-007_b.pdf

2:45pm - 5:10pm

MS-55(47b): Nanocrystalline materials II

Location: 223-4

Session Chair: Cinzia Giannini

Session Chair: Jinong Zhu

Introduction

2:45pm - 2:50pm

Introduction to session

[Cinzia Giannini](#), [Jinong Zhu](#)



MS-55(47b)-1786-001.pdf

2:50pm - 3:20pm

Picometer-level core-shell structure in Pd nanocrystals revealed by total scattering

[Kenichi Kato](#)^{1,2}, [Kazuya Shigeta](#)³, [Ryota Sato](#)⁴, [Miho Yamauchi](#)⁵, [Toshiharu Teranishi](#)⁴

¹RIKEN SPring-8 Center, Hyogo 679-5148, Japan; ²JST, PRESTO, Saitama 332-0012, Japan; ³Nippon Gijyutsu Center Co. Ltd, Hyogo 679-5148, Japan; ⁴Institute for Chemical Research, Kyoto University, Kyoto 611-0011, Japan; ⁵International Institute for Carbon-Neutral Energy Research (WPI-I2CNER), Kyushu University, Fukuoka 819-0395, Japan; katok@spring8.or.jp

External Resource:



MS-55(47b)-1081-002_b.pdf

3:20pm - 3:40pm

The journey from disorder to order: transformation of ferrite magnets investigated *in situ* by combined Bragg & total scattering analysis

[Priyank Shyam](#), [Harikrishnan Vijayan](#), [Mogens Christensen](#)

Aarhus University, Aarhus C, Denmark; priyank@inano.au.dk

External Resource:



MS-55(47b)-1311-003_b.pdf

3:40pm - 4:00pm

Millisecond structural dynamics during the piezoelectric cycle of silk fibroin by synchrotron X-ray scattering & comparison with DFT calculation

[Christopher Garvey](#)^{1,2}, [Stephen Mudie](#)³, [Denis Music](#)⁴, [Pär Olsson](#)^{4,5}, [Vitor Sencadas](#)⁶

¹Lund Institute for Advanced Neutron and X-ray Science, Lund 20503, Sweden; ²Heinz Maier-Leibnitz Zentrum (MLZ), Lichtenbergstrasse 1 85747, Garching, Germany; ³Australian Synchrotron, ANSTO, 800 Blackburn Rd, Clayton, 3168, Australia; ⁴Department of Materials Science and Applied Mathematics, Malmö University, SE-205 06 Malmö, Sweden; ⁵Division of Mechanics, Lund University, Box 118, 221 00 Lund, Sweden; ⁶School of Mechanical, Materials, Mechatronic and Biomedical Engineering, University of Wollongong, Wollongong, NSW, 2522, Australia; christopher.garvey@tum.de

External Resource:



MS-55(47b)-1180-004_b.pdf

4:00pm - 4:20pm

A high-throughput method for combinatorial screening of metal nanoparticles using x-ray pair distribution function analysis

[Songsheng Tao](#)¹, [Samira Shiri](#)², [Dan Kurtz](#)², [Nate James Cira](#)², [Bryan Hunter](#)², [Simon J. L. Billinge](#)^{1,3}

¹Department of Applied Physics and Applied Mathematics, Columbia University, New York, NY, USA; ²Rowland Institute, Harvard University, Cambridge, MA, USA; ³Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton, NY, USA; st3107@columbia.edu

External Resource:



MS-55(47b)-948-005_b.pdf

4:20pm - 4:40pm

Controlling crystallization pathways and kinetics in multiferroic Bi₂Fe₄O₉

[Andrea Kirsch](#)¹, [Niels Lefeld](#)², [Mathias Gogolin](#)², [Soham Banerjee](#)³, [Kirsten M. Ø. Jensen](#)¹

¹University of Copenhagen, Department of Chemistry, Universitetsparken 5, DK-2100 Copenhagen, Denmark; ²Universität Bremen, Institut für Anorganische Chemie und Kristallographie, Leobener Straße 7 /NW2, D-28359 Bremen, Germany; ³PETRA III, Deutsches Elektronen-Synchrotron (DESY), Notkestrasse 85, 22607, Hamburg, Germany; anki@chem.ku.dk

External Resource:



MS-55(47b)-963-006_b.pdf

4:40pm - 5:10pm

Atomic pair distribution function analysis of goethite and/or hydroxyapatite functionalized cyclodextrin nanosponges

Songsheng Tao¹, Che Randy Nangah^{2,3}, Ketcha Joseph Mbadcam², Josepha Foba Tendo⁴, Simon J. L. Billinge^{1,5}

¹Department of Applied Physics and Applied Mathematics, Columbia University, New York, NY 10027; ²Department of Inorganic Chemistry, University of Yaounde I, P.O. Box 812 Yaounde, Cameroon; ³Local Materials Promotion Authority (MIPROMALO), MINRESI, P.O. Box 2396 Yaounde, Cameroon.; ⁴Department of Chemistry, University of Buea, P.O. Box 63 Buea, Cameroon; ⁵Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton, NY 11973; r5nanga@yahoo.com

External Resource:



MS-55(47b)-328-007_b.pdf

2:45pm - 5:10pm

MS-56: Analysis of the fine structure in electron diffraction data

Location: Club H

Session Chair: Tatiana Gorelik

Session Chair: Xiaodong Zou

Invited: Paul Voyles (USA), Cheuk-Wai Tai (Sweden)

Introduction

2:45pm - 2:50pm

Introduction to session

Tatiana Gorelik, Xiaodong Zhu



MS-56-1787-001.pdf

2:50pm - 3:20pm

Approximate Rotational Symmetries in Electron Nanodiffraction from Amorphous Materials

Shuoyuan Huang, Carter Frances, Paul Voyles

University of Wisconsin-Madison, Madison, United States of America; paul.voyles@wisc.edu

External Resource:



MS-56-1181-002_b.pdf

3:20pm - 3:50pm

Local structure analysis by pair distribution function obtained from a TEM

Cheuk-Wai Tai

Stockholm University, Stockholm, Sweden; cheuk-wai.tai@mmk.su.se

External Resource:



MS-56-1393-003_b.pdf

3:50pm - 4:10pm

Quantitative analysis of diffuse electron scattering in the lithium-ion battery cathode material

$\text{Li}_{1.2}\text{Ni}_{0.13}\text{Mn}_{0.54}\text{Co}_{0.13}\text{O}_2$

Romy Poppe¹, Daphne Vandemeulebroucke¹, Reinhard B. Neder², Joke Hadermann¹

¹University of Antwerp, Department of Physics, Electron Microscopy for Materials Science (EMAT), Groenenborgerlaan 171, B-2020 Antwerp, Belgium; ²Friedrich-Alexander-Universität Erlangen-Nürnberg, Department of Physics, Institute of Condensed Matter Physics, Schloßplatz 4, 91054 Erlangen, Germany; romy.poppe@uantwerpen.be

External Resource:



MS-56-171-004_b.pdf

4:10pm - 4:30pm

High-Throughput Electron Diffraction Reveals a Hidden Novel Metal-Organic Framework

Meng Ge, Zehao Huang, Xiaodong Zou

Stockholm University, Stockholm, Sweden; gemeng733@gmail.com

External Resource:





MS-56-664-005_b.pdf

4:30pm - 4:50pm

Scanning Nano-Structure Electron Microscopy - Hidden Potential for Evolving Systems

Yevgeny Rakita^{1,2}, James L. Hart², Partha Pratim Das³, Stavros Nicolopoulos³, Sina Shahrezaei⁴, Suveen Nigel Mathaudhu⁴, Mitra L. Taheri², Simon J. L. Billinge^{1,5}

¹Department of Applied Physics and Applied Mathematics, Columbia University, New York, NY, USA; ²Department of Materials Science and Engineering, Johns Hopkins University, Baltimore, MD, USA; ³NanoMEGAS SPRL, Belgium; ⁴Department of Materials Science and Engineering, University of California Riverside, Riverside, CA, USA; ⁵Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton, NY, USA; yr2369@columbia.edu

External Resource:



MS-56-898-006_b.pdf

4:50pm - 5:10pm

Information theory based plane symmetry classifications: revealing pseudo-symmetries in the presence of noise

Peter Moeck

Portland State University, PORTLAND, Oregon, USA; pmoeck@pdx.edu

External Resource:



MS-56-117-007_b.pdf

SMS-4: Using crystallography for education during the pandemic

Location: **Club D**

Session Chair: **Oluwatoyin Asojo**

Invited: **Karsten Theis (USA)**

Introduction

2:45pm - 2:50pm

Introduction to session

Oluwatoyin Asojo



SMS-4-1838-001.pdf

2:50pm - 3:20pm

Adaptable virtual X-Ray laboratories for online teaching, learning, and authentic practice

Yakov Cherner¹, Oluwatoyin Asojo², Phillip Cherner³, Yi He⁴, Hamid Garmestani⁵

¹ATeL - Advanced Tools for e-Learning, Swampscott, United States of America; ²Hampton University, Hampton, VA, United States of America; ³Microsoft Corporation, Redmond, WA, United States of America; ⁴City University of New York, NYC, NY, United States of America; ⁵Georgia Institute of Technology, Atlanta, GA, United States of America; ycherne@atelearning.com

External Resource:



SMS-4-892-002_b.pdf

3:20pm - 3:50pm

Learning in 3D with Pymol and Proteopedia during a pandemic: enzyme catalysis and conformational change

Karsten W Theis, Roderico Acevedo

Westfield State University, Westfield, United States of America; ktheis@westfield.ma.edu

External Resource:



SMS-4-1330-003_b.pdf

3:50pm - 4:10pm

Teaching crystallography and X-ray diffraction online with MS Teams - experience

Radomír Kužel

Charles University, Faculty of Mathematics and Physics, Czech Republic; kuzel@karlov.mff.cuni.cz

External Resource:



SMS-4-102-004_b.pdf

2:45pm - 5:10pm

4:10pm - 4:30pm

Using Zoom Webinar to Teach Advanced Topics in Crystallography

Joseph D. Ferrara¹, **Simon Bates**¹, **Amanda Cochran**¹, **Mark Del Campo**¹, **Christian R. G6b**², **Florian KleemiB**³, **Pierre Le Maguer6s**¹, **Jeff Lengyel**⁴, **Mathias Meyer**⁵, **Horst Puschmann**⁶, **Keisuke Saito**¹, **Christian Sch6rmmann**², **Alexandra Stanley**², **Paul N. Swebston**¹, **Fraser White**², **Jakub Wojciechowski**²

¹Rigaku Americas Corp., The Woodlands, TX, USA; ²Rigaku Europe SE, Frankfurt, Germany; ³University of Regensburg, Regensburg, Germany; ⁴Cambridge Crystallographic Data Centre Inc, Boston, MA, USA; ⁵Rigaku Polska Sp. z o. o., Wroclaw, Poland; ⁶OlexSys Ltd, Durham, United Kingdom; joseph.ferrara@rigaku.com

External Resource:



[SMS-4-1193-005_b.pdf](#)

4:30pm - 4:50pm

COVID-proofing Biochemistry and engaging diverse students with Crystallography Research

Oluwatoyin Asojo

Hampton University, Hampton, United States of America; oluwatoyin.asojo@hamptonu.edu

External Resource:



[SMS-4-1324-006_b.pdf](#)

4:50pm - 5:10pm

Integrating a discovery based remote/hybrid crystallography lab module into an undergraduate teaching laboratory during the pandemic

Joe Tanski

Vassar College, Poughkeepsie, New York, United States of America; jtanski@vassar.edu

External Resource:



[SMS-4-1338-007_b.pdf](#)

SF-4: Software Fayre 4

Location: **221-2**

Session Chair: **Martin Lutz**

<http://www.cryst.chem.uu.nl/lutz/>

2:55pm - 3:40pm

Open slot

Martin Lutz

Utrecht University, Utrecht, Netherlands, The; m.lutz@uu.nl

3:40pm - 4:25pm

Atomic pair distribution function (PDF) in the cloud

Simon Billinge

Columbia University + Brookhaven Lab, New York, United States of America; sb2896@columbia.edu

External Resource:



4:25pm - 5:10pm

Advanced modeling of nanostructure from Atomic Pair Distribution Functions (PDFs) using DiffpyCMI on Windows 10

Simon Billinge

Columbia University + Brookhaven Lab, New York, United States of America; sb2896@columbia.edu

External Resource:



5:10pm - 5:55pm

Crystallography online by the Bilbao Crystallographic Server

Gemma de la Flor Martin¹, **Mois I. Aroyo**²

¹Karlsruhe Institute of Technology, Karlsruhe, Germany; ²University of the Basque Country, Spain; gemma.delaflo@kit.edu

External Resource:



2:55pm - 5:55pm

5:10pm - 6:10pm

Afternoon break 4: Poster session B2, exhibition, coffee/tea

Location: **Exhibition and poster area**

Poster - 23 Protein design: Protein design and engineering

Session Chair: **Sheena McGowan**

Session Chair: **Charlotte Uetrecht**

5:10pm - 6:10pm

Poster session abstracts

Radomir Kužel



Poster - 23 Protein design-1950-001.pdf

Engineering of protein nanocages for superlattice formation and nanoparticle encapsulation

Tobias Beck

University of Hamburg, Hamburg, Germany

External Resource: Presentation



Poster - 23 Protein design-1264-002_b.pdf

Structural characterization of the lid of lipase 2 of *Pseudomonas alcaligenes*

Elena Lizbeth García-Villegas¹, Enrique Rudiño-Piñera², Liliana Pardo²

¹Centro de Investigación en Dinámica Molecular, UAEM, Cuernavaca, Morelos, Mexico; ²Instituto de Biotecnología, UNAM, Cuernavaca, Morelos, Mexico; liz.garcia@gmail.com

External Resource: Presentation



Poster - 23 Protein design-799-003_b.pdf

Structural and functional studies of key enzyme (LpxC (UDP-3-O-acyl-N-acetylglucosamine deacetylase) from *salmonella typhi* involved in Gram-negative bacterial lipid A biosynthesis

Sudhir Kumar Pal

vellore institute of technology, Vellore, India; sudhirkumarpal001@gmail.com

External Resource: Presentation



Poster - 23 Protein design-211-004_b.pdf

Crystallographic and biophysical studies of interactions of new β -lactoglobulin variants with tricyclic drugs

Paulina Wróbel¹, Joanna Loch¹, Piotr Bonarek², Krzysztof Lewiński¹

¹Jagiellonian University, Faculty of Chemistry, Department of Crystal Chemistry and Crystal Physics, Gronostajowa 2, 30-387 Krakow, Poland; ²Jagiellonian University, Faculty of Biochemistry, Biophysics and Biotechnology, Department of Physical Biochemistry, Gronostajowa 7, 30-387 Krakow, Poland

External Resource: Presentation



Poster - 23 Protein design-1417-005_b.pdf

SAKE: Computationally Designed Modular Protein Building Blocks for Macromolecular Assemblies

Staf M. L. Wouters¹, David E. Clarke^{1,2}, Hiroki Noguchi¹, Steven De Feyter², Arnout R. D. Voet¹

¹Laboratory of Biomolecular Modeling and Design, Department of Chemistry, KU Leuven, Celestijnenlaan 200G, 3001 Heverlee, Belgium; ²Division of Molecular Imaging and Photonics, Department of Chemistry, KU Leuven, Celestijnenlaan 200F, 3001 Heverlee, Belgium

External Resource: Presentation



Poster - 23 Protein design-1598-006_b.pdf

Poster - 24 Crystallization: Crystallization

Session Chair: Duane Choquesillo-Lazarte



5:10pm - 6:10pm

Poster session abstracts

Radomír Kužel



Poster - 24 Crystallization-1951-001.pdf

A novel sample delivery system based on circular motion for serial crystallography

Feng-Zhu Zhao, Xiao-Qian Jin, Liang-Liang Chen, Da-Chuan Yin

Northwestern Polytechnical University, Xi'an, China, People's Republic of

External Resource: Presentation



Poster - 24 Crystallization-1167-002_b.pdf

Dynamic theory of protein crystallization

Jindřich Hašek

Czech Academy of Sciences, Institute of Biotechnology, Průmyslová 595, Vestec, 252 50, Czech Republic

External Resource:



Poster - 24 Crystallization-802-003_b.pdf

Nucleation and growth of a single suspended protein crystal by merging phase separated droplets

Da-Chuan Yin, Zi-Qing Wu, Yong-Ming Liu

Northwestern Polytechnical University, Xi'an, China, People's Republic of



Poster - 24 Crystallization-1232-004_b.pdf

Preparation of hemoglobin crystals of desired size

Xiaoqian Jin, Fengzhu Zhao, Renbin Zhou, Dachuan Yin

Northwestern Polytechnical University, Xi'an, China, People's Republic of

External Resource:



Poster - 24 Crystallization-1208-005_b.pdf

Batch crystallisation methods for serial crystallography experiments

John H. Beale, May E. Sharpe

Paul Scherrer Institut, Villigen-PSI, Switzerland

External Resource:



Poster - 24 Crystallization-1169-006_b.pdf

Exploring Structural Implications of diphosphinamine ligands in Medicine and Catalysis

Dumisani Kama¹, Alice Brink¹, Roger Alberto², Andreas Roodt¹

¹University of the Free State; ²University of Zürich; tomkama112@gmail.com

External Resource:



Poster - 24 Crystallization-878-007_b.pdf

Combining RMC and PDF methods to characterize amorphous drug

Vinicius Danilo Nonato Bezzon¹, João Cardoso de Lima², Fabio Furlan Ferreira¹

¹Federal University of ABC, Santo André - SP, Brazil; ²Federal University of Santa Catarina, Florianópolis - SC, Brazil; vinicius.bezzon@gmail.com

External Resource:



Poster - 24 Crystallization-985-008_b.pdf

Halogenated rhodium(I) complexes as model catalysts for methanol carbonylation.

Lerato Bosman, Alice Brink, Dumisani Kama

University of the Free State, Bloemfontein, South Africa; leratobosman1@gmail.com

External Resource:



Poster - 24 Crystallization-651-009_b.pdf

Reactivity, bonding and structural elucidation of pendant methyl-pyridinato β -diketiminato ligand moiety

Sanjukta Pahar, Sakya S. Sen

CSIR-NATIONAL CHEMICAL LABORATORY, Pune, India; sanjuktaapahar@gmail.com

External Resource:



Poster - 24 Crystallization-1032-010_b.pdf

5:10pm - 6:10pm

Poster - 25 Electron: Electron crystallography

Session Chair: **Petr Brazda**



Poster session abstracts

Radomír Kužel



Poster - 25 Electron-1952-001.pdf

Dynamical refinement of beam sensitive crystals: going below a total dose of 0.1 e⁻/Å²

Holger Klein, Emre Yörük, Stéphanie Kodjikian

Institut Néel, Grenoble, France; holger.klein@neel.cnrs.fr

External Resource:



Poster - 25 Electron-810-002_b.pdf



Poster - 25 Electron-810-002_c.pdf

An electron diffractometer : A novel device for electron crystallography experiments

Gunther Steinfeld, Arianna E. Lanza, Eric Hovestreydt, Gustavo Santiso-Quinones

ELDICO Scientific AG, 5234 Villigen, Switzerland; steinfeld@eldico.ch

External Resource:



Poster - 25 Electron-828-003_b.pdf

Synergy ED: A new electron diffractometer for microED

Fraser White¹, Akihito Yamano¹, Sho Ito¹, Takashi Matsumoto¹, Hiroyasu Sato¹, Joseph Ferrara², Mathias Meyer³, Michał Jasnowski³, Eiji Okunishi⁴, Yoshitaka Aoyama⁴

¹Rigaku Corporation, Haijima, Tokyo, Japan; ²Rigaku Americas Corporation, The Woodlands, Texas, USA; ³Rigaku Polska, Wrocław, Poland; ⁴JEOL Ltd., Akishima, Tokyo, Japan; fraser.white@rigaku.com

External Resource:



Poster - 25 Electron-1118-004_b.pdf

The 'Why' and 'How' of a Dedicated Electron Diffractometer

Eric Hovestreydt, Arianna Lanza, Gunther Steinfeld, Gustavo Santiso-Quinones

ELDICO Scientific AG, 5234 Villigen, Switzerland; hovestreydt@eldico.ch

External Resource:



Poster - 25 Electron-599-005_b.pdf

Ab initio structure determination of two new titanium phosphates synthesized via molten salt synthesis.

Hilke Petersen¹, Niklas Stegmann¹, Michael Fischer^{2,3}, Bodo Zibrowius¹, Wolfgang Schmidt¹, Martin Etter⁴, Claudia Weidenthaler¹

¹Max-Planck-Institut für Kohlenforschung, Heterogeneous Catalysis, Kaiser-Wilhelm-Platz 1 45470 Mülheim, Germany;

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Poster - 25 Electron-1055-006_b.pdf

Effect of nano-SiC doping on the structure and superconducting properties of Mg (B_{1-x}C_x)₂

Mauro Melone^{1,2}, Cesar Sobrero³, Horacio Troiani^{2,4}, María Teresa Malachevsky^{2,4}, Adriana Serquis^{1,4}

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⁴Comisión Nacional de Energía Atómica, Av. Bustillo 9500 Bariloche, Argentina; mauro.m.melone@gmail.com

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Poster - 25 Electron-1615-007_b.pdf

Investigating structure transformations of $\text{La}_x\text{Sr}_{2-x}\text{MnO}_{4-\delta}$ using *in situ* 3D electron diffraction in a gas environment

Daphne Vandemeulebroucke, Maria Batuk, Joke Hadermann

1EMAT, University of Antwerp, Groenenborgerlaan 171, B-2020 Antwerp, Belgium; daphne.vandemeulebroucke@uantwerpen.be

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Poster - 25 Electron-1400-008_b.pdf

Investigating nanoparticle surface energetics using 4D-STEM

Bryan David Esser^{1,2}, Alison M Funston³, Joanne Etheridge^{1,2}

¹Monash Centre for Electron Microscopy, Monash University, VIC, 3800, Australia; ²Department of Materials Engineering, Monash University, VIC, 3800, Australia; ³School of Chemistry, Monash University, VIC, 3800, Australia; bryan.esser@monash.edu

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Poster - 25 Electron-1161-009_b.pdf

Simulation of electron diffraction patterns of organic crystals under continuous rotation

Tarik Ronan Drevon

STFC, London, United Kingdom; tarik.drevon@stfc.ac.uk

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Poster - 25 Electron-1440-010_b.pdf

The perks of a Zeiss Libra 120 plus TEM - First steps towards electron diffraction

Christoph Grininger¹, Gerhard Hofer², Hongyi Xu², Xiaodong Zou², Tea Pavkov-Keller¹

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Poster - 25 Electron-1618-011_b.pdf

Machine Learning Calculation of Large Angle Convergent Beam Electron Diffraction Patterns

Richard Beanland

University of Warwick, Coventry, United Kingdom; r.beanland@warwick.ac.uk

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Poster - 25 Electron-1680-012_b.pdf

Refinement on electron diffraction data in MoPro: A quest for improved structure model

Kunal Kumar Jha¹, Barbara Gruza¹, Michal Chodkiewicz¹, Christian Jelsch², Paulina Dominiak¹

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Poster - 25 Electron-1890-013_b.pdf

Poster - 26 Spectroscopy: Combining X-Ray Diffraction and Spectroscopy to Characterise Materials

Session Chair: **Carlo Meneghini**

Session Chair: **Siegbert Schmid**

Poster session abstracts

Radomír Kužel

5:10pm - 6:10pm





Poster - 26 Spectroscopy-1953-001.pdf

Structure of ferroelectric low temperature phase of yttrium manganate YMn_2O_5 revisited

Tina Weigel¹, Carsten Richter², Melanie Nentwich³, Matthias Zschornak¹, Dirk C. Meyer¹

¹TU Bergakademie Freiberg, Freiberg, Germany; ²Leibniz-Institut für Kristallzüchtung, Berlin, Germany; ³DESY Photon Science, Deutsches Elektronensynchrotron, Hamburg, Germany; tina.weigel@physik.tu-freiberg.de

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Poster - 26 Spectroscopy-1410-002_b.pdf

Exploiting the complementarity between X-ray scattering and absorption techniques to investigate breast cancer metastasis

Andre L. C. Conceição¹, Sylvio Haas², Volkmar Müller⁵, Eike Burandt³, Malte Mohme⁴

¹DESY, Hamburg, Germany; ²DESY, Hamburg, Germany; ³Universitätsklinikum Hamburg-Eppendorf, Martinistraße 52, D-20246 Hamburg, Germany; ⁴Universitätsklinikum Hamburg-Eppendorf, Martinistraße 52, D-20246 Hamburg, Germany; ⁵Universitätsklinikum Hamburg-Eppendorf, Martinistraße 52, D-20246 Hamburg, Germany; andre.conceicao@desy.de

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Poster - 26 Spectroscopy-743-003_b.pdf

Refractory materials structural and surface changes by sulfuric acid treatment

Enida Nushi¹, Lorenci Gjurgjaj², Altin Mele^{1,2}

¹Ivodont Academy, Tirane, Albania; ²Faculty of Natural Sciences, University of Tirana; enida.nushi@ivodont.org

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Poster - 26 Spectroscopy-398-004_b.pdf

Ferroelectricity driven by 'A' and 'B' site off-centered displacements in cubic phase with Pm-3m space group

DIGVIJAY NATH DUBEY¹, GURVINDERJIT SINGH², SAURABH TRIPATHI¹

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Poster - 26 Spectroscopy-642-005_b.pdf

Synthesis and structural resolution by X-ray diffraction of polycrystalline samples of (E)-N-benzylidene-4-haloanilines

Laura Díaz^{1,2,3}, Angy Katherin Soto Navarro^{1,2,3}, José Antonio Henao^{1,2}, Robert Toro^{1,2}, Juan Manuel Urbina González^{1,3}

¹Universidad Industrial de Santander, Bucaramanga, Colombia; ²Grupo de Investigación en Química Estructural (GIQUE), UIS Guatiguará, Km 2 vía Refugio, 681011, Piedecuesta, Colombia; ³Laboratorio de Química Orgánica y Biomolecular (LQOBio), Escuela de Química, Universidad Industrial de Santander; LAURA.DIAZ14@correo.uis.edu.co

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Poster - 26 Spectroscopy-417-006_b.pdf



Poster - 26 Spectroscopy-417-006_c.pdf

Vibrational spectroscopy as a confirmation method for structural analysis

A. S. Abdel-Rahman¹, S. Kamal Abdel-Aal¹, Gyula Faigel², Katalin Kamaras², Bortel Gábor², Arron Pekker²

¹Physics department, Faculty of Science, Cairo University, Egypt; ²Institute for Solid State Physics and Optics, Wigner Research Centre for Physics, Hungary; asabry@sci.cu.edu.eg

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Poster - 26 Spectroscopy-400-007_b.pdf

Poster - 27 Magnetism: Magnetic structures, magnetic materials



5:10pm - 6:10pm

Poster session abstracts

Radomír Kužel



Poster - 27 Magnetism-1954-001.pdf

INVESTIGATION OF THE VIABILITY OF STRUCTURAL INFORMATION DETERMINED WITH X-RAY DIFFRACTION EMPLOYED TO DETERMINE ANISOTROPIC MAGNETIC SUSCEPTIBILITY

Rasmus Degn

Aarhus University, Aarhus, Denmark; 201404329@post.au.dk



Poster - 27 Magnetism-956-002_b.pdf

The magnetic materials beamlines at Diamond Light Source

Dan Porter

Diamond Light Source Ltd, Didcot, United Kingdom; dan.porter@diamond.ac.uk

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Poster - 27 Magnetism-242-003_b.pdf

Symmetry breaking and Optical property of high-temperature superconductor $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$

Kun Zhang¹, Masataka Matsumoto², Kenta Nakagawa^{3,4}, Azusa Matsuda¹, Genki Shiro⁵, Toru Asahi^{1,6,7}

¹Department of Advanced Science and Engineering, Waseda University, Tokyo, Japan; ²Department of Mathematics, Shanghai University, Shanghai, China; ³Kanagawa Institute of Industrial Science and Technology (KISTEC), Ebina, Japan; ⁴Department of Applied Physics and Physico-Informatics, Keio University, Yokohama, Japan; ⁵Department of Biophysics, Kyoto University, Kyoto, Japan; ⁶Waseda Research Institute for Science and Engineering, Waseda University, Tokyo, Japan; ⁷Global Consolidated Research Institute for Science Wisdom, Waseda University, Tokyo, Japan; zk19941123@ruri.waseda.jp

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Poster - 27 Magnetism-1249-005_b.pdf

Magnetic Structures of RNiSi_3 (R = Gd, Tb and Ho)

Rodolfo Tartaglia¹, Fabiana Rodrigues Arantes², Carlos William Galdino¹, Danilo Rigitano¹, Ulisses Ferreira Kaneko³, Marcos de Abreu Avila², Eduardo Granado¹

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Poster - 27 Magnetism-548-006_b.pdf

Non-collinear magnetic order coupled with magnetic glassy behaviour and enhancement of magnetocaloric effect under high pressure

SRIKANTA GOSWAMI¹, Babu P D¹, Rajeev Rawat²

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Poster - 27 Magnetism-213-007_b.pdf

Magnetic properties and magnetic structure of the quasi one-dimensional antiferromagnet $\text{Cu}_2(\text{MoO}_4)(\text{SeO}_3)$

Pharit Piyawongwatthana¹, Kazuhiro Nawa¹, Stuart A Calder², Daisuke Okuyama¹, Taku J Sato¹

¹IMRAM, Tohoku University, Sendai, Japan; ²Neutron Scattering Division, Oak Ridge National Laboratory, USA; piyawongwatthana.pharit.p3@dc.tohoku.ac.jp

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Poster - 27 Magnetism-1138-008_b.pdf



Poster - 27 Magnetism-1138-008_c.pdf

Hyperfine interactions of ^{57}Fe nuclei in a weak ferromagnet FeBO_3

Nikita Snegirev¹, Sergey Starchikov¹, Igor Lyubutin¹, Ekaterina Smirnova¹, Mikhail Chuev², Sergey Yagupov³, Mark Strugatsky³, Olga Alekseeva¹

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Poster - 27 Magnetism-628-009_b.pdf

Synthesis and characterization of mullite-type NdMnTiO₅: structural, spectroscopic, thermogravimetric and magnetic properties analyses

Kowsik Ghosh¹, M. Mangir Murshed^{1,3}, Debabrata Nayak¹, Thomas Frederichs², Thorsten M. Gesing^{1,3}

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²University of Bremen, Faculty of Geosciences, D-28359 Bremen, Germany; ³MAPEX Center for Materials and Processes, Bibliothekstraße 1, Universität Bremen, D-28359 Bremen, Germany; ghosh@uni-bremen.de

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Poster - 27 Magnetism-361-010_b.pdf

Rare-earth dodecaborides: still cubic or not?

Olga N. Khrykina¹, Alexander P. Dudka¹, Nadezhda B. Bolotina¹, Natalya Yu. Shitsevalova², Nikolay E. Sluchanko³

¹FSRC "Crystallography and Photonics" RAS, Moscow, Russian Federation; ²Institute for Problems of Materials Science, NASU, Kyiv, Ukraine; ³Prokhorov General Physics Institute, RAS, Moscow, Russian Federation; kvarkpower@gmail.com

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Poster - 27 Magnetism-230-011_b.pdf

Frustrated magnets with chemically tailorable interactions

Alasdair J. Bradford^{1,2}, Wenjiao Yao¹, Ivan de Silva³, Mark Telling³, Tatiana Guidi³, Manh Duc Li³, Stephen L. Lee², Philip Lightfoot¹

¹School of Chemistry, University of St Andrews, St Andrews, United Kingdom; ²School of Physics and Astronomy, University of St Andrews, St Andrews, United Kingdom; ³ISIS Neutron and Muon Source, STFC RAL, Didcot, UK; ajb35@st-andrews.ac.uk

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Poster - 27 Magnetism-226-012_b.pdf

One-dimensional coordination polymers based on cobalt(II) and nickel(II)

Ana Karina Seguin^{1,2}, Carlos Cruz^{1,2}, Diego Venegas-Yazigi^{2,3}, Verónica Paredes-García^{1,2}

¹Andres Bello, Departamento de Ciencias Químicas, Santiago, Chile; ²Centro para el Desarrollo de la Nanociencia y Nanotecnología, CEDENNA, Santiago, Chile; ³Departamento de Ciencia de los Materiales, Universidad de Santiago de Chile, Santiago, Chile; vparedes@unab.cl

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Poster - 27 Magnetism-951-013_b.pdf

Structural and magnetic investigations of post-perovskite thiocyanate frameworks

Madeline Geers^{1,2}, Laura Cañadillas Delgado², Oscar Fabelo², Matthew Cliffe¹

¹School of Chemistry, University of Nottingham, University Park, Nottingham, NG7 2RD, UK; ²Institut Laue-Langevin, 71 Avenue des Martyrs, CS 20156, 38042 Grenoble Cedex 9, FRANCE; geers@ill.fr

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Poster - 27 Magnetism-1465-014_b.pdf

Magnetic aspects and assemblies of solvent-mediated layered manganese dicarboxylate based coordination polymers

Bharti Singh¹, Madhulika Mazumdar², Balendra .1, Sundaresan Athinarayanan², Swapan Kumar Pati², Arunachalam Ramanan^{*1}

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Poster - 27 Magnetism-1681-015_b.pdf

Crystal structure and magnetism in $\text{Nd}_{1-x}\text{Sr}_x\text{FeO}_3$ ($0.1 \leq x \leq 0.9$)

Charles Herve Marie Hervoches¹, Hiroshi Nakatsugawa²

¹Nuclear Physics Institute, v.v.i., CAS, Řež, Czech Republic; ²Yokohama National University, Japan; hervoches@ujf.cas.cz

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Poster - 27 Magnetism-1876-016_b.pdf

Intermetallic compounds containing f-elements: synthesis of some of the compounds from the system R_2TGe_6 (R=Dy, Er; T=Ni, Cu, Pd)

Cinthia Antunes Corrêa^{1,2}, Markéta Jarošová¹, António Pereira Gonçalves³, Margarida Sousa Henriques¹

¹Academy of Sciences of the Czech Republic, Prague, Czech Republic; ²Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic; ³Instituto Superior Técnico, Universidade de Lisboa, Portugal; correa@fzu.cz

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Poster - 27 Magnetism-1495-017_b.pdf



Poster - 27 Magnetism-1495-017_c.pdf

Poster - 28 Porous: Porous materials

Session Chair: Karena Chapman

Session Chair: Fernando Uribe-Romo



5:10pm - 6:10pm

Poster session abstracts

Radomír Kužel



Poster - 28 Porous-1955-001.pdf

Low-dose imaging of metal-organic frameworks and study of their electron-beam stability

Asma Mansouri¹, Georges Mouchaham¹, Gilles Patriarche², Christian Serre¹

¹Institut des matériaux poreux de Paris, Ecole normale supérieure, ESPCI, CNRS, PSL University, Paris, France; ²Center for Nanoscience and Nanotechnology, C2N UMR 9001, CNRS, Université Paris Sud, Université Paris Saclay, Palaiseau, France; asma.mansouri@ens.psl.eu

External Resource:  Presentation



Poster - 28 Porous-1374-002_b.pdf

Biophysical and preliminary crystallographic studies of Lectin from Entada rheedii seeds

Sanjay Naik

Vellore Institute of Technology (VIT), Vellore, India; sharmasanjay459@gmail.com

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Poster - 28 Porous-300-003_b.pdf

Ternary coordination compounds of copper with amino acids and 1,10-phenanthroline –structural insight and biological activity

Biserka Prugovečki, Darko Vušak, Katarina Ležaić, Mia Jurković

Faculty of Science, University of Zagreb, Zagreb, Croatia; biserka@chem.pmf.hr

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Poster - 28 Porous-1497-004_b.pdf

Use of alkylarsonium cations as probe molecules for the study of zeolites

J. L. Jorda¹, S. Saez-Ferre¹, Ch. W. Lopes^{1,2}, J. Simancas¹, A. Vidal-Moya¹, T. Blasco¹, G. Agostini³, G. Minguez-Espallargas⁴, F. Rey¹, P. Oña-Burgos¹

¹Instituto de Tecnología Química (UPV-CSIC) Universitat Politècnica de València-Consejo Superior de Investigaciones Científicas, Valencia, SPAIN; ²LRC, Institute of Chemistry, Universidade Federal do Rio Grande do Sul, Porto Alegre, BRAZIL; ³ALBA Synchrotron Light Facility, Cerdanyola del Vallés, Barcelona, SPAIN; ⁴Instituto de Ciencia Molecular (ICMo), Universitat de València, Paterna, SPAIN; jjorda@itq.upv.es

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Poster - 28 Porous-1480-005_b.pdf

Adsorption of perfluorooctanoic acid (PFOA) and perfluorooctane sulfonate (PFOS) emerging contaminants on Y and silver-Y exchanged zeolites using thermal analysis and X-ray diffraction facilities.

Maura Mancinelli, Francesco Colombo, Matteo Ardit, Annalisa Martucci

Department of Physics and Earth Sciences, University of Ferrara, Via Saragat 1, I-44121, Ferrara, Italy; mncmra1@unife.it



Poster - 28 Porous-916-006_b.pdf

Application of the Crystalline Sponge Method for Structure Determination of Persistent Organic Pollutants of Agrochemical Degradation Products

Takashi Kikuchi¹, Kazuhiro Takagi², Futa Sakakibara³, Takashi Sato¹

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Poster - 28 Porous-1527-007_b.pdf

Breathing Mixed-ligand MOFs – solvent exchange and sorption studies

Nabanita Chatterjee, Nolwazi Gcwensa, Clive Lloyd Oliver

University of Cape Town, Rondebosch, South Africa; clive.oliver@uct.ac.za

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Poster - 28 Porous-1925-008_b.pdf

Poster - 29 Solid state: Solid state reactions and dynamics

Session Chair: **Javier Marti-Rujas**

Session Chair: **Franziska Emmerling**



5:10pm - 6:10pm

Poster session abstracts

Radomír Kužel



Poster - 29 Solid state-1956-001.pdf

In-situ time-resolved X-ray diffraction studies of crystalline materials under static mechanical load

Valentin Akkuratov^{1,2}, Eliovich Yan^{1,2}, Targonskiy Anton^{1,2}, Pisarevsky Yuri^{1,2}, Blagov Alexander^{1,2}, Kovalchuk Michail^{1,2}

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Poster - 29 Solid state-531-002_b.pdf

Synthesis and crystal growth of Rh(IV) oxides with double perovskite structure

Holub Tamara

IFW Dresden, Dresden, Germany; t.holub@ifw-dresden.de



Poster - 29 Solid state-843-003_b.pdf

Single crystal to single crystal transformations in Co(II) dynamic framework

Christelle Noelle Dzesse Tekouo^{1,2,3}, Emmanuel Ngwang Nfor², Susan Ann Bourne³

¹Department of Mineral Engineering, School of Chemical Engineering and Mineral Industries, Ngaoundere, University of Ngaoundere;

²Department of Chemistry, University of Buea, Buea, Cameroon; ³Department of Chemistry Centre for Supramolecular Chemistry Research University of Cape Town Rondebosch South Africa 7701; christellencelle12@gmail.com

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Poster - 29 Solid state-287-004_b.pdf

Structure and Reactivity of Rhodium(I) Carbonyl complexes as Model Nano-Wired Assemblies and Catalyst

Pennie Petrus Mokolokolo, Marietjie Schutte-Smith, Alice Brink, Andreas Roodt
University of the Free State, Bloemfontein, South Africa; mokolokolopp@ufs.ac.za

External Resource:  Presentation



Poster - 29 Solid state-837-005_b.pdf

Synthesis, crystal structure and catalytic oxidation studies of a new acid pyrophosphate metallate

Najlaa HAMDI, Mohamed AKOUIBAA, Rim Ben ali cherif, Brahim EL BALI, Mohammed LACHKAR
Faculty of Sciences, FES, Morocco; hamdi.najlae@gmail.com

External Resource:  Presentation



Poster - 29 Solid state-405-006_b.pdf

Thin layer formation in TeO₂ single crystals due to migration of charge carriers

Anton Kulikov^{1,2}, Alexander Blagov^{1,2}, Nikita Marchenkov^{1,2}, Alexander Ilin³, Yury Pisarevsky^{1,2}, Mikhail Kovalchuk^{1,2}

¹National Research Center "Kurchatov Institute", pl. akademika Kurchatova 1, Moscow, Russian Federation; ²Shubnikov Institute of Crystallography of Federal Scientific Research Centre "Crystallography and Photonics" Russian Academy of Sciences, Leninsky prospekt 59, Moscow, Russian Federation; ³Physics Department, Lomonosov Moscow State University, Leninskie Gory 1-2, Moscow, Russian Federation; antonik@gmail.com

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Poster - 29 Solid state-415-007_b.pdf

Photothermal high-speed crystal actuation and the simulation

Shodai Hasebe¹, Yuki Hagiwara¹, Jun Komiya¹, Meguya Ryu², Hiroki Fujisawa³, Junko Morikawa³, Tetsuro Katayama⁴, Daiki Yamanaka⁴, Akihiro Furube⁴, Hiroyasu Sato⁵, Toru Asahi^{1,6}, Hideko Koshima⁶

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External Resource:  Presentation



Poster - 29 Solid state-1251-008_b.pdf

Poster - 30 Nano: Nanomaterials

Session Chair: **Cinzia Giannini**
Session Chair: **Jinong Zhu**



5:10pm - 6:10pm

Poster session abstracts

Radomir Kužel



Poster - 30 Nano-1957-001.pdf

Sc doped TiO₂ nanocrystals with core-shell morphology

Snejana Bakardjieva¹, Victor Zenou^{2,3}

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External Resource:  Presentation



Poster - 30 Nano-1373-002_b.pdf

Combined structural and electrical characterization of zirconia-based thin films for energy applications

Y. Mansilla¹, M. Arce^{1,2}, C. E. Jiménez², J. Basbus¹, D. M. Többsen², A. Serquis¹

¹INN-CNEA-CONICET, Av. Bustillo 9500, S. C. de Bariloche, Rio Negro, 8400, Argentina; ²Helmholtz-Zentrum Berlin für Materialien und Energie, Albert-Einstein-Str.15, 12489, Berlin, Germany; mansillayanet@gmail.com

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Poster - 30 Nano-1065-003_b.pdf

Understanding the gas sensing mechanism in vanadium doped tin oxides using X-ray diffraction and X-ray photoelectron spectroscopy

Nirman Chakraborty, Ambarish Sanyal, Sagnik Das, Debdulal Saha, Samar Kumar Medda, Swastik Mondal
CSIR Central Glass and Ceramic Research Institute, KOLKATA, India; nirmanchakraborty910@gmail.com

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Poster - 30 Nano-308-005_b.pdf

Grafen/CNT doped polymer based nano composites: RF Shielding properties of the nano composite coated fabric materials.

Mustafa Zafer Belirgen¹, Gözde Bayazit Sekitmen¹, Semra İde²

¹Department of Nanotechnology and Nanomedicine, Hacettepe University, Beytepe, Ankara 06800, Turkey; ²Department of Physics Engineering, Hacettepe University, Beytepe, Ankara 06800, Turkey; belirgen.zafer@gmail.com

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Poster - 30 Nano-602-006_b.pdf



Poster - 30 Nano-602-006_c.pdf

Preparation and Characterization of Pd modified TiO₂ nanofiber catalyst for carbon-carbon coupling Heck reaction

Dickson Andala¹, Leah Nyangasi², Charles Onindo²

¹Multimedia University of Kenya, Nairobi, Kenya; ²Kenyatta University, Kenya; andalad@gmail.com



Poster - 30 Nano-167-007_b.pdf

Impact of Co²⁺ substitution on microstructural evolution and magnetic properties of zinc ferrite nanoparticles synthesized by precipitation and hydrothermal-joint method

Mohammed S. M. Abdelbaky¹, Ahmed M. Abu-Dief^{1,2}, Santiago García-Granda¹

¹Departments of Physical and Analytical Chemistry, and Organic and Inorganic Chemistry University of Oviedo-CINN, 33006 Oviedo;

²Chemistry Department, Faculty of Science, Sohag University, 82524 Sohag, Egypt; saidmohammed.uo@uniovi.es

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Poster - 30 Nano-1048-008_b.pdf

High-purity crystalline silicon gels

Samantha L. Flores-Lopez², Lucia dos Santos-Gomez¹, Natalia Rey-Raap¹, **Santiago Garcia-Granda**¹, Ana Arenillas²

¹University of Oviedo, Oviedo, Spain; ²Instituto de Ciencia y Tecnología del Carbono, INCAR-CSIC, Oviedo, Spain; sgg@uniovi.es

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Poster - 30 Nano-872-009_b.pdf

Structure identification of Fe-Fe_xO_y core shell nanoparticles and their time stability

Tereza Vaclavu¹, Jan Filip², Daniel Niznansky³, Michal Vaclavu¹, Jan Endres¹, Milan Dopita¹, Stanislav Danis¹

¹Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic; ²Regional centre of advanced technologies and materials, Olomouc, Czech Republic; ³Faculty of Science, Charles University, Prague, Czech Republic; vaclavut@centrum.cz

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Poster - 30 Nano-1732-010_b.pdf



Poster - 30 Nano-1732-010_c.pdf

A novel electrolytic method of preparing Nano sized α-Ferric oxide from scrap iron

Prabal Dasgupta, Elias Tadesse, **Ismail Kamil**, Adem Ahmed

Jimma University, Ethiopia, Jimma, Ethiopia; jilalokamil1@gmail.com

External Resource:





Poster - 30 Nano-1537-011_b.pdf

Impacts of mutual phase interactions on piezoelectric and dielectric properties

Kun-Ta Lin, Chia-Hung Pan, Wet-ting Li, Jr-jeng Ruan

National Cheng Kung University, Tainan, Taiwan; s153126@gmail.com

External Resource:



Poster - 30 Nano-1866-012_b.pdf

Growth and stability of SmS-TaS₂ nanotubes studied by XAFS and DAFS methods.

Azat Khadiev¹, Madhenahalli-Bhyrappa Sreedhara², Reshef Tenne², Dmitri Novikov¹

¹Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany; ²Weizmann Institute of Science, Rehovot, Israel; azat.khadiev@desy.de

External Resource:



Poster - 30 Nano-1866-013_b.pdf

Fast Debye equation calculation on graphics processing units - GPU used for calculation and fitting of nanoparticles real structure

Milan Dopita¹, Lukáš Horák¹, Václav Holý¹, Martin Rudolph²

¹Charles University, Prague, Czech Republic; ²TU Bergakademie Freiberg, Germany; dopita@gmail.com

External Resource:



Poster - 30 Nano-1886-014_b.pdf

Poster - 31 Total: Total scattering

Session Chair: **Emil Bozin**

Session Chair: **Pierre Bordet**



5:10pm - 6:10pm

Poster session abstracts

Radomír Kužel



Poster - 31 Total-1958-001.pdf

Temperature and composition evolution of lattice, charge density wave and superconducting orders in Ta-based dichalcogenides by total x-ray scattering

Valeri Petkov

Central Michigan University, Mount Pleasant, United States of America; petko1vg@cmich.edu

External Resource:



Poster - 31 Total-707-002_b.pdf

Single-crystal total scattering meets metal-organic frameworks: deciphering the elusive structure of ZIF-90

Stefano Canossa¹, Ruggero Frison², Xiaokun Pei³, Hans-Beat Bürgi⁴

¹University of Antwerp; ²University of Zurich; ³University of California Berkeley; ⁴University of Bern; stefano.canossa@uantwerpen.be

External Resource:



Poster - 31 Total-871-003_b.pdf

PDF Analysis of Crystalline and Amorphous Materials on a Home Laboratory Diffractometer

Joseph Ferrara¹, Pierre Le Maguerès¹, Christian Schürmann², Mathias Meyer³, Jakub Wojciechowski², Simon Bates¹

¹Rigaku Americas Corp, The Woodlands, United States of America; ²Rigaku Europe SE, Frankfurt, Germany; ³Rigaku Polska Sp. z o. o, Wrocław, Poland; joseph.ferrara@rigaku.com

External Resource:





Poster - 31 Total-1050-004_b.pdf

Implementation for coping with sample and instrument effects for reverse Monte Carlo modelling of total scattering data

Yuanpeng Zhang

Oak Ridge National Laboratory, Knoxville, United States of America; zhangy3@ornl.gov

External Resource:



Poster - 31 Total-755-005_b.pdf

Studying local order in ferroelectric oxide superlattices with three-dimensional diffuse X-ray scattering

Joohee Bang^{1,2}, Nives Strkalj^{1,2}, Martin Sarott¹, Morgan Trassin¹, Thomas Weber¹

¹Department of Materials Science, ETH Zurich, Zurich, Switzerland; ²Department of Materials Science and Metallurgy, Cambridge University, United Kingdom; joohee.bang@mat.ethz.ch

External Resource:



Poster - 31 Total-1530-006_b.pdf

Characterization of C-S-H gels by pair distribution function analysis

Ana Cuesta, Alejandro Morales-Cantero, Angeles G. De la Torre, Isabel Santacruz, Miguel A.G. Aranda

Universidad de Malaga, Malaga, Spain; g_aranda@uma.es

External Resource:



Poster - 31 Total-1454-007_b.pdf

5:10pm - 6:10pm

Poster - 32 Theory: Theoretical crystallography



Poster session abstracts

Radomír Kužel



Poster - 32 Theory-1959-001.pdf

Algebraic analysis of topological domain-interface defects in crystals

James H. McKenzie, Branton J. Campbell

Brigham Young University, Provo, United States of America; james.mck28@gmail.com

External Resource:



Poster - 32 Theory-1072-002_b.pdf

Local structure representation beyond symmetry constraints: Glazer tilts in perovskites

Sandra H. Skjaervog, Simon J. L. Billinge

Columbia University, New York; sandraskj@gmail.com

External Resource:



Poster - 32 Theory-1539-003_b.pdf



Poster - 32 Theory-1539-003_c.pdf

A comparative research between atomic-based and chemical calculation-based descriptor for cocrystal screening machine learning model

Yingquan Hao, Ying-Chieh Hung, Yusuke Shimoyama

Tokyo Institute of Technology, Tokyo, Japan; yshimo@chemeng.titech.ac.jp

External Resource:



Poster - 32 Theory-1493-004_b.pdf

SPECIFIC WATER STRUCTURE IN A GEO-INSPIRED NANOTUBE AND INTERRELATED DYNAMICS

Geoffrey Monet¹, Arianna D'Angelo^{1,2}, Erwan Paineau¹, Gilberto teobaldi³, Stéphane Rois², Pascale Launois¹
¹Laboratoire de Physique des Solides, CNRS, université Paris-Saclay, Orsay, France; ²Institut Laue-Langevin, Grenoble, France;
³STFC, Daresbury laboratory, UK; pascale.launois@universite-paris-saclay.fr

External Resource:  Presentation



Poster - 32 Theory-786-005_b.pdf

Dynamical effects in the integrated X-ray scattering intensity from single crystals with microdefects in Bragg diffraction geometry

Sergey Dmitriev, Vadim Molodkin, Stepan Olikhovskii, Vyacheslav Lizunov
 1G.V. Kurdyumov Institute for Metal Physics, N.A.S. of Ukraine, Kyiv, Ukraine; dsv2003@ukr.net

External Resource:  Presentation



Poster - 32 Theory-1346-006_b.pdf

Result of using atoms and centrosymmetric cubic space groups

Pui Sum Yuen
 Nil, HONG KONG, Hong Kong S.A.R. (China); puisumyuen@netvigator.com

External Resource:  Presentation



Poster - 32 Theory-1670-007_b.pdf

Determination of structure of CoS₂ by the means of a simple new method; a solution to the phase problem for centrosymmetric cubic crystals

Pui Sum Yuen
 Nil, HONG KONG, Hong Kong S.A.R. (China); puisumyuen@netvigator.com

External Resource:  Presentation



Poster - 32 Theory-1855-008_b.pdf

6:10pm - 7:00pm

KN-19: X-ray absorption spectroscopy and materials science: recent advances

Location: **Terrace 2A**
 Session Chair: **Giuliana Aquilanti**
Federico Boscherini

X-ray absorption spectroscopy and materials science: recent advances

Federico Boscherini
 University of Bologna, Bologna, Italy; federico.boscherini@unibo.it

External Resource:  Presentation



KN-19-1363-001_b.pdf

6:10pm - 7:00pm

KN-20: The benefits of Scanning Precession Electron Diffraction to access to the crystallographic phases and orientations of nanomaterials

Location: **Terrace 2B**
 Session Chair: **Louisa Meshi**
Edgar Rauch

The benefits of Scanning Precession Electron Diffraction to access to the crystallographic phases and orientations of nanomaterials

Edgar F Rauch
 University Grenoble Alpes - CNRS, Saint Martin d'Hères, France; edgar.rauch@simap.grenoble-inp.fr

External Resource:  Presentation



KN-20-1326-001_b.pdf

6:10pm - 7:00pm

KN-21: How limitless antibodies are generated by V(D)J recombination

Location: **Club A**
 Session Chair: **Marcin Nowotny**
Wei Yang

How limitless antibodies are generated by V(D)J recombination

Wei Yang¹, Xuemin Chen¹, Min-sung Kim², Martin Gellert¹

External Resource:



KN-21-152-001_b.pdf

8:00pm - 10:00pm **Boat trip: Boat trip with raut**
Extra fee
More



Date: Thursday, 19/Aug/2021

9:00am - 9:50am **KN-22: Record High superconductivity in sodalite-like rare-earth hydrides stabilized at high pressures**
Location: **Terrace 2A**
Session Chair: **Arthur Haozhe Liu**
Yanming Ma



Clathrate Superhydrides Under High Pressure Conditions: A Class of Extraordinarily Hot Conventional Superconductors

Yanming Ma

College of Physics, Jilin Univ., Changchun 130012, China; mym@jlu.edu.cn

External Resource:



KN-22-1269-001_b.pdf

9:00am - 9:50am **KN-23: Novel insights on biomineralization using x-rays and optical coherent diffraction based imaging**
Location: **Terrace 2B**
Session Chair: **Juan Manuel Garcia-Ruiz**
Virginie Chamard



Novel insights on biomineralization using x-rays and optical coherent diffraction based imaging approaches

Virginie Chamard

Aix-Marseille Univ, CNRS, Centrale Marseille, Institut Fresnel, Marseille, France; virginie.chamard@fresnel.fr

External Resource:



KN-23-1427-001_a.doc



KN-23-1427-001_b.pdf

9:00am - 9:50am **KN-24: Regulation of gene expression by transcription factors and RNA-binding proteins**
Location: **Club A**
Session Chair: **Pavčina Řezáčová**
Udo Heinemann



Regulation of gene expression by transcription factors and RNA-binding proteins

Udo Heinemann

Max Delbrück Center for Molecular Medicine, Berlin, Germany; heinemann@mdc-berlin.de

External Resource:



KN-24-1436-001_b.pdf

9:50am - 10:20am **Morning break 5: Posters, coffee/tea**
Location: **Exhibition and poster area**

10:20am - 12:45pm **MS-57: Neutron scattering - sources, applications**
Location: **Terrace 2B**
Session Chair: **Matthew Paul Blakeley**
Session Chair: **Flora Meilleur**
Session Chair: **Esko Oksanen**



Invited: **Gloria Borgstahl (USA)**, **Svetlana Antonyuk (UK)**

Introduction

10:20am - 10:25am

Introduction to session

Matthew Paul Blakeley, Flora Meilleur, Esko Oksanen



MS-57-1788-001.pdf

10:25am - 10:55am

Direct detection of concerted proton and electron transfer in human manganese superoxide dismutase

Gloria Borgstahl¹, Jahaun Azadmanesh¹, Will Lutz¹, Kevin Weiss², Leighton Coates²



¹University of Nebraska Medical Center, Omaha, Nebraska, United States of America; ²Oak Ridge National Laboratory, Tennessee, United States of America

External Resource:  Presentation



MS-57-197-002_b.pdf

10:55am - 11:25am

Damage-free structures of green copper nitrite reductase obtained by neutron crystallography and XFEL

Svetlana Antonyuk

Molecular Biophysics Group, ISMIB, Faculty of Health and Life Sciences; University of Liverpool, UK

External Resource:  Presentation



MS-57-1375-003_b.pdf

11:25am - 11:45am

Modelling and refinement of hydrogens: new developments in CCP4

Lucrezia Catapano^{1,2}, Roberto A. Steiner¹, Garib N. Murshudov²

¹King's College London, London, United Kingdom; ²MRC Laboratory of Molecular Biology, Cambridge, United Kingdom;

lucrezia.catapano@kcl.ac.uk

External Resource:  Presentation



MS-57-1016-004_b.pdf

11:45am - 12:05pm

Finding the Goldilocks zone for chemical crystallography via Laue single-crystal neutron diffraction – what have we learned from KOALA to improve KOALA 2.0?

Alison Jeanine Edwards, Ross Oliver Piltz

ANSTO, Lucas Heights, Australia; Alisonedwar@gmail.com

External Resource:  Presentation



MS-57-1295-005_b.pdf

12:05pm - 12:25pm

An automatised hydrogen orientation procedure for neutron protein crystallography

Justin Bergmann¹, Esko Oksanen², Ulf Ryde¹

¹Division of Theoretical Chemistry, Lund University, Chemical Centre, P.O. Box 124, SE-221 00 Lund, Sweden; ²European Spallation Source ESS ERIC, Lund, Sweden

External Resource:  Presentation



MS-57-813-006_b.pdf

12:25pm - 12:50pm

Amplifying hydrogen: neutron diffraction using Dynamic Nuclear Polarization

Dean Myles¹, Josh Pierce¹, Mathew Cuneo², Kenneth Herwig¹, Flora Meilleur^{1,3}, Jinkui Zhao⁴

¹Oak Ridge National Laboratory, Oak Ridge, United States of America; ²St. Jude Children's Research Hospital, Memphis, United States of America; ³North Carolina State University, Raleigh, United States of America; ⁴Institute of Physics, Chinese Academy of Sciences, Beijing, China



MS-57-1685-007_b.pdf

MS-58: Ultra-high resolution macromolecular crystallography and quantum biocrystallography

Location: **Club A**

Session Chair: **Christian Jelsch**

Session Chair: **Alexander Wlodawer**

Invited: **Paulina Dominiak (Poland), Maciej Kubicki (Poland)**

Introduction

10:20am - 10:25am

Introduction to session

Christian Jelsch, Alexander Wlodawer



MS-58-1789-001.pdf

10:20am - 12:45pm

10:25am - 10:55am

Experimental studies of the details of electron density distribution in a Z-DNA hexamer: new insights, new problems

Maciej Kubicki¹, Krzysztof Brzezinski², Benoit Guillot³, Mariusz Jaskolski^{1,2}, Zbigniew Dauter⁴

¹Faculty of Chemistry, Adam Mickiewicz University in Pozna, Poznan, Poland; ²Institute of Bioorganic Chemistry, Polish Academy of Sciences, Poznan, Poland; ³Laboratoire de Cristallographie, Institut Jean Barriol, Université de Lorraine, Nancy, France; ⁴Macromolecular Crystallography Laboratory, National Cancer Institute, Argonne National Laboratory, Argonne, USA

External Resource:



MS-58-751-002_b.pdf

10:55am - 11:25am

Moving quantum crystallography from sub-atomic XRD to near-atomic 3D ED

Paulina Maria Dominiak, Michał Leszek Chodkiewicz, Barbara Gruza, Kunal Kumar Jha, Marta Kulik, Paulina Rybicka, Aleksandra Sypko

Biological and Chemical Research Centre, Department of Chemistry, University of Warsaw, Warszawa, Poland

External Resource:



MS-58-1378-003_b.pdf

11:25am - 11:50am

Principles of the mechanism of interfacial activation of a lipase: open and closed states and lipid – enzyme interactions in the limbus region of *Candida antarctica* Lipase B

Michele Cianci

Università Politecnica Delle Marche, Ancona, Italy

External Resource:



MS-58-1059-004_b.pdf

11:50am - 12:15pm

Investigating the redox cycle of tryptaredoxin at ultra-high resolution

Martin Streit, **Hermann Schindelin**

University of Würzburg, Würzburg, Germany

External Resource:



MS-58-1308-005_b.pdf

12:15pm - 12:40pm

Theoretical electrostatic potential maps of macromolecules calculated with multipolar electron scattering factors

Marta Kulik, Michał Leszek Chodkiewicz, Paulina Maria Dominiak

Biological and Chemical Research Centre, Department of Chemistry, University of Warsaw, Warsaw, Poland

External Resource:



MS-58-638-006_b.pdf

MS-59: Crystal chemistry with emerging technology I

Location: **Terrace 2A**

Session Chair: **Consiglia Tedesco**

Session Chair: **Toru Asahi**

Invited: **Sota Sato** (Japan), **Marijana Dakovic** (Croatia)

Introduction

10:20am - 10:25am

Introduction to session

Consiglia Tedesco, **Toru Asahi**



MS-59-1790-001.pdf

10:25am - 10:55am

Functional crystalline materials based on macrocyclic nanochannels

Sota SATO

Department of Applied Chemistry, The University of Tokyo, Tokyo, Japan; satosota@appchem.t.u-tokyo.ac.jp

10:20am - 12:45pm

External Resource:



MS-59-582-002_b.pdf

10:55am - 11:25am

Variable adaptability of coordination polymers of cadmium(II) to external mechanical stimuli

Marijana Đaković, Mateja Pisačić

University of Zagreb, Zagreb, Croatia; mdjakovic@chem.pmf.hr

External Resource:



MS-59-968-003_b.pdf

11:25am - 11:45am

In situ photoswitching of spirorhodamines isomers in solid-state

Julietta Alday¹, Mateo Michel Torino¹, Lucia Alvarez², Maria Gabriela Lagorio¹, Cristian Huck Iriart³, Sebastian Suarez¹

¹Buenos Aires University, CABA, Argentina.; ²IIB, UNSAM, 25 de mayo y Francia, San Martín Buenos Aires, Argentina.; ³ECyT, UNSAM, 25 de mayo 1169, San Martín, Buenos Aires, Argentina.; sebasuarez85@gmail.com

External Resource:



MS-59-162-004_b.pdf

11:45am - 12:05pm

The pancake-bonding of semiquinone radicals under variable pressure and temperature conditions.

Nikita Bogdanov^{1,2}, Valentina Milašinović³, Boris Zakharov^{1,2}, Elena Boldyreva^{1,2}, Krešimir Molčanov³

¹Borisev Institute of Catalysis SB RAS, Novosibirsk, Russia; ²Novosibirsk State University, Novosibirsk, Russia; ³Ruder Bošković Institute, Zagreb, Croatia; nebo1329@gmail.com

External Resource:



MS-59-1397-005_b.pdf

12:05pm - 12:25pm

Structural chemistry of azulenes

Nick Gerasimchuk¹, Mikhail Barybin²

¹Missouri State University, Springfield, Missouri, United States of America; ²University of Kansas, Lawrence, Kansas, United States of America; NNGerasimchuk@MissouriState.edu

External Resource:



MS-59-885-006_b.pdf

12:25pm - 12:45pm

Understanding the role of non-covalent interactions in the acridine with different acids of salt molecules

SUGANYA SURESH¹, SARAVANAN KANDASAMY², KUMARADHAS POOMANI¹

¹Laboratory of Biocrystallography and Computational Molecular Biology Department of Physics, Periyar University, Salem-636 011, India; ²Faculty of Chemistry, University of Warsaw, Warsaw-02093, Poland; convey2sugan@gmail.com

External Resource:



MS-59-993-007_b.pdf

MS-60: Composite and incommensurate modulated crystals: structural and physical properties

Location: Club B

Session Chair: Sylvain Ravy

Session Chair: Sander van Smaalen

Invited: Stephan J. Skinner (UK), Vincent Jacques (France)

Introduction

10:20am - 10:25am

Introduction to session

Sylvain Ravy, Sander van Smaalen

10:20am - 12:45pm



MS-60-1791-001.pdf

10:25am - 10:55am

Investigating the modulated structures in the $\text{La}(\text{Nb,W})\text{O}_{4+d}$ family of oxide ion conductors

Stephen John Skinner¹, **Cheng Li**², **Stevin Pramana**³

¹Imperial College London, London, United Kingdom; ²Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA; ³School of Engineering, Newcastle University, UK; s.skinner@imperial.ac.uk

External Resource:



MS-60-154-002_b.pdf

10:55am - 11:25am

Revealing pinning and solitonic transport of sliding charge-density-waves by coherent and nano-XRD

Vincent Jacques

CNRS / Laboratoire de Physique des Solides, Orsay, France; vincent.jacques@u-psud.fr

External Resource:



MS-60-1438-003_b.pdf

11:25am - 11:45am

Polytelluride Anions in Deficient $\text{RETe}_{2-\delta}$ Structures – Superstructures and Bonding Analysis

Hagen Poddig, **Kati Finzel**, **Thomas Doert**

Technische Universität Dresden, Dresden, Germany; hagen.poddig@tu-dresden.de

External Resource:



MS-60-656-004_b.pdf

11:45am - 12:05pm

Hysteretic structural changes within five-layered modulated 10M martensites of Ni-Mn-Ga(-Fe)

Petr Vertát^{1,2}, **Ladislav Straka**¹, **Hanuš Seiner**³, **Alexei Sozinov**⁴, **Milan Klicpera**⁵, **Oscar Fabelo**⁶, **Oleg Heczko**¹

¹Institute of Physics of the Czech Academy of Sciences, Na Slovance 1999/2, 18221 Prague 8, Czech Republic; ²Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University in Prague, Trojanova 13, 12000 Prague 2, Czech Republic; ³Institute of Thermomechanics of the Czech Academy of Sciences, Dolejškova 1402/8, 18200 Prague 8, Czech Republic; ⁴Material Physics Laboratory, LUT University, Yliopistonkatu 34, 53850 Lappeenranta, Finland; ⁵Faculty of Mathematics and Physics, Charles University, Ke Karlovu 5, 12116 Prague 2, Czech Republic; ⁶Institut Laue-Langevin, 71 avenue des Martyrs, CS 20156, 38042 Grenoble cedex 9, France; vertat@fzu.cz

External Resource:



MS-60-1216-005_b.pdf

12:05pm - 12:25pm

The interplay of framework instability and electron-phonon coupling in a CDW system, the monophosphate tungsten bronze family.

Arianna Minelli¹, **Elen Duverger-Nedellec**², **Alain Pautrat**³, **Olivier Pérez**³, **Marc De Boissieu**⁴, **Marek Mihalkovic**^{5,6}, **Alexei Bosak**⁷, **Andrew Goodwin**¹

¹University of Oxford, Oxford, United Kingdom; ²CMCB, CNRS, Université de Bordeaux, UMR 5026, F-33600 Pessac, France; ³Laboratory CRISMAT, UMR 6508 CNRS, ENSICAEN 6 Boulevard du Marechal Juin, F-14050 Caen Cedex 4, France; ⁴Institute of Physics, Slovak Academy of Sciences, Dúbravská cesta 9, Bratislava 84511, Slovak Republic; ⁵Université Grenoble Alpes, SIMaP, F-38000 Grenoble, France; ⁶CNRS, SIMaP, F-38000 Grenoble, France; ⁷European Synchrotron Radiation Facility, 6 rue Jules Horowitz, F-38000 Grenoble, France; arianna.minelli@chem.ox.ac.uk

External Resource:



MS-60-525-006_b.pdf

12:25pm - 12:45pm

$\text{Ba}_{10}\text{Y}_6\text{Ti}_4\text{O}_{27}$ an aperiodic oxide with an unusually low thermal conductivity.

John Bleddyn Claridge

University of Liverpool, Liverpool, United Kingdom; j.b.claridge@liv.ac.uk

External Resource:





MS-60-1115-007_b.pdf

MS-61: Magnetic structures at extreme conditions and in extreme samples



Location: **Club D**

Session Chair: **Angel M. Arevalo-Lopez**

Session Chair: **Andrzej Katrusiak**

Invited: **Elena Solana-Madruga (UK), Dawid Pinkowicz (Poland)**

Introduction

10:20am - 10:25am

Introduction to session

Angel M. Arevalo-Lopez, Andrzej Katrusiak



MS-61-1792-001.pdf

10:25am - 10:55am



Complex magnetic structures in frustrated A-site manganites

Elena Solana-Madruga

1CNRS, Université de Lille, Unité de Catalyse et chimie du Solid, 59652 Villeneuve d'Ascq Cedex, France;

elena.solanamadruga@univ-lille.fr

External Resource:



MS-61-845-002_b.pdf

10:55am - 11:25am



High pressure effects in molecular magnetic materials with cyanide bridges

Dawid Pinkowicz

Jagiellonian University, Faculty of Chemistry, Krakow, Poland; dawid.pinkowicz@uj.edu.pl

External Resource:



MS-61-1496-003_b.pdf

11:25am - 11:45am



Crystal and magnetic structures of the high pressure RMnMnTaO₆ (R = Rare earth) double (double) perovskites

Kunlang Ji, Gessica Moyo, J. Paul Attfield

CSEC and School of Chemistry, University of Edinburgh; kij2@ed.ac.uk

External Resource:



MS-61-832-004_b.pdf

11:45am - 12:05pm



Pb₂NiOsO₆: antiferromagnetic order breaks inversion symmetry in high pressure perovskite

Emma E. McCabe¹, Hai L. Feng², Chang-Jong Kang³, Pascal Manuel⁴, Fabio Orlandi⁴, Yu Su⁵, Jie Chen⁵, Yoshihiro Tsujimoto⁵, Joke Hadermann⁶, Gabriel Kotliar³, Kazunari Yamaura⁵, Martha Greenblatt²

¹Durham University, Durham, United Kingdom; ²Department of Chemistry and Chemical Biology, Rutgers, the State University of New Jersey, Piscataway, New Jersey 08854, United States; ³Department of Physics and Astronomy, Rutgers, the State University of New Jersey, Piscataway, New Jersey 08854, United States; ⁴ISIS Facility, STFC, Rutherford Appleton Laboratory, Didcot, Oxfordshire OX11 0QX, U.K.; ⁵International Center for Materials Nanoarchitectonics (WPI-MANA), National Institute for Materials Science, Tsukuba, Ibaraki 305-0044, Japan; ⁶EMAT, University of Antwerp, 2020 Antwerp, Belgium; emma.mccabe@durham.ac.uk

External Resource:



MS-61-1408-005_b.pdf

12:05pm - 12:25pm



High Pressure Diffraction on Single Crystals with Hot Neutrons at MLZ

Martin Meven^{1,2}, Andrzej Grzechnik¹, Vladimir Hutanu^{1,2}, Karen Friese³, Andreas Eich^{1,3}, Georg Roth¹

¹Institute of Crystallography, RWTH Aachen University, 52056 Aachen, Germany; ²Jülich Centre for Neutron Science at Heinz Maier-Leibnitz Zentrum, Forschungszentrum Jülich GmbH, 85747 Garching, Germany; ³Jülich Centre for Neutron Science-2/Peter Grünberg-Institute-4, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany; martin.meven@frm2.tum.de

External Resource:





MS-61-865-006_b.pdf

12:25pm - 12:45pm

Magnetic phase diagram of the high-temperature spiral magnet YBaCuFeO₃



Jike Lyu¹, Tian Shang^{1,2}, Mickaël Morin^{1,3}, María Teresa Fernández-Díaz⁴, Marisa Medarde¹

¹Paul Scherrer Institut, Villigen, Switzerland; ²Laboratory for Multiscale Materials Experiments, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland; ³Excelsus Structural Solutions (Swiss) AG, PARK innovAARE, 5234 Villigen, Switzerland; ⁴Institut Laue Langevin, 71 avenue des Martyrs, CS 20156, 38042 Grenoble CEDEX 9, France; jike.lyu@psi.ch

External Resource:



MS-61-1187-007_b.pdf

MS-62: The mineral/life interface - prebiotic chemistry, biomineralization, advanced biomimetic materials



Location: **Club C**

Session Chair: **Juan Manuel Garcia-Ruiz**

Session Chair: **Giuseppe Falini**

Invited: **Boaz Pokroy** (Israel), **Abel Moreno** (Mexico)

Introduction

10:20am - 10:25am

Introduction to session



Juan Manuel Garcia-Ruiz, Giuseppe Falini



MS-62-1793-001.pdf

10:25am - 10:55am

Incorporation of amino acids into inorganic crystalline hosts: from biomineralization to bio-Inspired band gap engineering



Boaz Pokroy

Technion Israel Institute of Technology, Haifa, Israel; bpokroy@technion.ac.il

External Resource:



MS-62-1376-002_b.pdf

10:55am - 11:25am

The role of intramineral proteins involved into the biomineralization of calcium carbonate in eggshells formation. Implications to the dinosaurs' extinction



Abel MORENO, Nerith Rocío ELEJALDE-CADENA

Instituto de Química. Universidad Nacional Autónoma de México, Mexico City, Mexico; carcamo@unam.mx

External Resource:



MS-62-1490-003_b.pdf

11:25am - 11:45am

Crystal texture of mineral self-organized structures from soda lake water and their implication to early Earth and prebiotic chemistry



Melese Getenet, Juan Manuel Garcia-Ruiz

Laboratorio de Estudios Cristalográficos, Instituto Andaluz de Ciencias de la Tierra, Consejo Superior de Investigaciones Científicas–Universidad de Granada, Granada, Spain; dessie.melese@csic.es

External Resource:



MS-62-327-004_b.pdf

11:45am - 12:05pm

Structure and properties of coralline red alga: from helical configuration to alternating layers



Nuphar Bianco-Stein, Iryna Polishchuk, Boaz Pokroy

Technion, Haifa, Israel; piryna@technion.ac.il

External Resource:



MS-62-1432-005_b.pdf

10:20am - 12:45pm

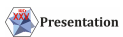
12:05pm - 12:25pm

Non-destructive 3D orientational mapping of bone using diffractive X-ray tomography

Fredrik K. Mürer¹, Sophie Sanchez², Kristin Olstad³, Marco Di Michiel⁴, Basab Chattopadhyay¹, Dag W. Breiby^{1,5}

¹PoreLab, Department of Physics, Norwegian University of Science and Technology (NTNU), Høgskoleringen 5, 7491 Trondheim, Norway; ²Uppsala University, Department of Organismal Biology, Evolutionary Biology Centre, Norbyvägen 18 A, 75236, Uppsala, Sweden.; ³Faculty of Veterinary Medicine, Department of Companion Animal Clinical Sciences, Norwegian University of Life Sciences, Oslo, Norway.; ⁴ESRF-The European Synchrotron, 71 Avenue des Martyrs, 38000 Grenoble, France.; ⁵Department of Microsystems, University of South-Eastern Norway (USN), Campus Vestfold, 3184 Borre, Norway.; fredrik.k.murer@ntnu.no

External Resource:



MS-62-1114-006_b.pdf

MS-63: Catalysis: functionalized materials studied by XRD and XAFS

Location: **223-4**

Session Chair: **Valérie Briois**

Session Chair: **Andreas Roodt**

Invited: **Elisa Borfecchia (Italy)**, **Ola F Wendt (Sweden)**

Introduction

10:20am - 10:25am

Introduction to session

Valerie Briois, Andreas Roodt



MS-63-1794-001.pdf

10:20am - 12:45pm

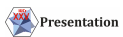
10:25am - 10:55am

Heterogenization of molecular catalysts: C–H activation and dehydrogenation

Ola F. Wendt

Lund University, LUND, Sweden; ola.wendt@chem.lu.se

External Resource:



MS-63-182-002_b.pdf

10:55am - 11:25am

Understanding local structure and redox chemistry of metal ions in nanoporous catalysts by X-ray absorption spectroscopy

Elisa Borfecchia

University of Turin, Turin, Italy; elisa.borfecchia@unito.it

External Resource:



MS-63-913-003_b.pdf

11:25am - 11:45am

XAS and XRD analysis of active Pt and Pd sites in metal-organic framework UiO-67

Alina Skorynina¹, Aram Bugaev¹, Kirill Lomachenko², Alexander Guda¹, Andrea Lazzarini³, Unni Olsbye³, Karl Petter Lillerud³, Alexander Soldatov¹

¹Southern Federal University, Rostov-on-Don, Russian Federation; ²ESRF, Grenoble, France; ³University of Oslo, Oslo, Norway; alinaskorynina@gmail.com

External Resource:



MS-63-290-004_b.pdf

11:45am - 12:05pm

Structural dynamics of nanoalloy catalysts for Fuel Cells by *in situ* total x-ray scattering

Valeri Petkov

Central Michigan University, Mount Pleasant, United States of America; petko1vg@cmich.edu

External Resource:



MS-63-706-005_b.pdf

12:05pm - 12:25pm

The Hopeful Journey Towards Successful Tailoring Of Water (In)Soluble Cobalt Analogues As Potential Water Splitting Catalysts.

Orbett Alexander¹, Roger Alberto², Andreas Roodt¹

¹Dept. of Chemistry, University of the Free State, Bloemfontein, 9300, South Africa; ²Dept. of Chemistry, University of Zürich, Winterthurerstrasse 190, Zürich, Switzerland.; alexanderorbett@gmail.com

External Resource:  Presentation



MS-63-413-006_b.pdf

12:25pm - 12:45pm

Structural and bandgap modification of KLaTiO₄ hydrogen evolution catalyst

Junwei Ben Li, Brendan J. Kennedy, Christopher D. Ling, Thomas Maschmeyer
The University of Sydney, Sydney, Australia; juli0440@uni.sydney.edu.au

External Resource:  Presentation



MS-63-764-007_b.pdf

MS-64: In-situ and time resolved electron crystallography

Location: Club H

Session Chair: **Andrew Alexander Stewart**

Session Chair: **Eva Olsson**

Invited: **David Flannigan (USA)**, **Maria Batuk (Belgium)**

Introduction

10:20am - 10:25am

Introduction to session

Andrew Alexander Stewart, Eva Olsson



MS-64-1795-001.pdf

10:25am - 10:55am

Following structure evolution of SrFeO_x in redox reactions using *in situ* 3D electron diffraction

Maria Batuk, Daphne Vandemeulebroucke, Joke Hadermann
EMAT, University of Antwerp, Antwerp, Belgium; maria.batuk@uantwerpen.be

External Resource:  Presentation



MS-64-1228-002_b.pdf

10:55am - 11:25am

Time-resolved TEM beyond fast detectors

David J. Flannigan, Jialiang Chen, Wyatt Curtis, Daniel X. Du, Paige E. Engen, Elisah J. VandenBussche, Yichao Zhang
Department of Chemical Engineering and Materials Science, University of Minnesota, 421 Washington Avenue SE, Minneapolis, Minnesota 55455, United States of America; flan0076@umn.edu

External Resource:  Presentation



MS-64-889-003_b.pdf

11:25am - 11:50am

Time resolved x-ray diffraction studies of prospective crystalline materials under dynamic ultrasonic loads

Yan Eliovich^{1,2}, Anton Targonskiy^{1,2}, Alexander Blagov^{1,2}, Yuri Pisarevsky^{1,2}, Valentin Akkuratov^{1,2}, Andrei Protsenko^{1,2}, Michail Kovalchuk^{1,2}

¹FSRC "Crystallography and photonics" RAS, Moscow, Russian Federation; ²NRC "Kurchatov Institute", Moscow, Russian Federation; yan.eliovich@gmail.com

External Resource:  Presentation



MS-64-476-004_a.pdf

11:50am - 12:15pm

Discovering and transforming precipitate phases in aluminium alloys using *in situ* transmission electron microscopy

Laure Bourgeois^{1,2}, Zezhong Zhang^{3,4}, Yong Zhang², Xiaofen Tan², Yiqiang Chen⁵, Matthew Weyland^{1,2}, Philip N.H. Nakashima², Nikhil V. Medhekar²

¹Monash Centre for Electron Microscopy, Monash University, Australia; ²Department of Materials Science and Engineering, Monash University, Australia; ³Electron Microscopy for Materials Research, University of Antwerp, Belgium; ⁴Department of Materials, University of Oxford, UK; ⁵ThermoFisher Scientific, The Netherlands; laure.bourgeois@monash.edu

External Resource:  Presentation



MS-64-824-005_b.pdf

12:15pm - 12:40pm

Elucidation of Linker Motion in Metal-Organic Frameworks by Three-Dimensional Electron Diffraction

Laura Samperisi¹, Aleksander Jaworski¹, Gurpreet Kaur¹, Karl P. Lillerud², Xiaodong Zou¹, Zhehao Huang¹

¹stockholm university, stockholm, Sweden; ²University of Oslo, Oslo, Norway; laura.samperisi@mmk.su.se

External Resource:



MS-64-727-006_b.pdf

12:45pm - 2:45pm

Lunch 5: Posters, lunches

Location: **Exhibition and poster area**

ECA - GIG-1: ECA - GIG-1 Young Crystallographers

Location: **Club A**

[Link](#)

1:00pm - 2:30pm

ECA - SIG-12: ECA - SIG-12 Crystallography of Functional Materials

Location: **223-4**

[Link](#)

1:00pm - 2:30pm

ECA - SIG-1: ECA - SIG-1 Macromolecular Crystallography

Location: **Club D**

[Link](#)

1:00pm - 2:30pm

ECA - SIG-3: ECA - SIG-3 Aperiodic Crystals

Location: **virtual**

[Link](#)

1:00pm - 2:30pm

ECA - SIG-5: ECA - SIG-5 Mineral and Inorganic Crystallography

Location: **Club B**

SIG - 5

1:00pm - 2:30pm

ECA - SIG-6: ECA - SIG-6 Instrumentation and Experiment

Location: **Club C**

[Link](#)

1:00pm - 2:30pm

Meeting - Quantum: Commission on Quantum Crystallography Open Meeting

Location: **Club H**

Session Chair: **Paulina Maria Dominiak**

Video: **Intro - Sagamore - Bodensteiner**

1:00pm - 2:30pm

ECA - SIG-4: ECA - SIG-4 Electron Crystallography

Location: **221-2**

[Link](#)

1:45pm - 2:45pm

ECA - GIG-3: ECA - GIG-3 Education in Crystallography

Location: **virtual**

[Link](#)

2:00pm - 2:45pm

MS-65: Graphs, tilings and crystal structures

Location: **Club D**

Session Chair: **Mark Loyola**

Session Chair: **Bernd Souvignier**

Invited: **Vladislav A. Blatov (Russia), Jean-Guillaume Eon (Brazil)**

[Introduction](#)

2:45pm - 2:50pm

Introduction to session

Mark Loyola, Bernd Souvignier

2:45pm - 5:10pm



MS-65-1796-001.pdf

2:50pm - 3:20pm

Perceiving zeolite self-assembly within the natural tiling model

Vladislav A. Blatov^{1,2}

¹Samara Center for Theoretical Materials Science (SCTMS), Samara National Research University, Samara, Russian Federation;

²Samara Center for Theoretical Materials Science (SCTMS), Samara State Technical University, Samara, Russian Federation;

blatov@topospro.com

External Resource:



MS-65-224-002_b.pdf

3:20pm - 3:50pm

Combinatorial aspects of Löwenstein's rule

Jean-Guillaume Eon¹, Montauban Moreira de Oliveira Jr²

¹Federal University of Rio de Janeiro, Rio de Janeiro, Brazil; ²Rural Federal University of Rio de Janeiro; jgeon@ig.ufrj.br

External Resource:



MS-65-573-003_b.pdf

3:50pm - 4:15pm

Layer Groups associated with 3-way 3-fold isonemal fabrics

Kristan B. Liza, Ma. Louise Antonette N. De Las Penas

Ateneo De Manila University, Quezon City, Philippines; kristan.liza@obf.ateneo.edu

External Resource:



MS-65-334-004_b.pdf

4:15pm - 4:40pm

A unique and continuous code of all periodic crystals

Vitaliy Kurlin, Olga Anosova, Daniel Widdowson

University of Liverpool, Liverpool, United Kingdom; vitaliy.kurlin@liverpool.ac.uk

External Resource:



MS-65-867-005_b.pdf



MS-65-867-005_c.pdf

4:40pm - 5:05pm

Synthesis of magnetically frustrated oxides with double perovskite structure

Anastasia Smerechuk^{1,2}, Ryan Morrow¹, Sabine Wurmehl¹, Oleg Sidletskiy²

¹Institute for Solid-State and Materials Research, Dresden, Germany; ²Institute for Scintillation Materials NAS of Ukraine, Kharkiv, Ukraine; a.smerechuk@ifw-dresden.de

External Resource:



MS-65-945-006_b.pdf

MS-66: Integrative structural biology: The next 50 years of the Protein Data Bank

Location: **Club H**

Session Chair: **Stephen K. Burley**

Session Chair: **Dina Schneidman**

Invited: **Andrej Sali** (USA), **Fei Xu** (China)

Introduction

2:45pm - 2:50pm

Introduction to session

Stephen K. Burley, **Dina Schneidman**



MS-66-1797-001.pdf

2:50pm - 3:20pm

Crystal structure of the first orphan GPCR

Fei Xu

ShanghaiTech University, Shanghai, China, People's Republic of



MS-66-746-002_b.pdf

3:20pm - 3:50pm

From integrative structural biology to cell biology

Andrej Sali

University of California, San Francisco, San Francisco, United States of America

External Resource:



MS-66-666-003_b.pdf

3:50pm - 4:10pm

Crystal and Cryo-EM structures provide insight into how pro-neurodegenerative SARM1 is activated and cleave NAD⁺.

Thomas Ve¹, Weixi Gu², Jeffrey D. Nanson², Yun Shi², Katie Cunnea³, Philip S. Kerry³, Todd Bosanac⁴, Robert O. Hughes⁴, Bostjan Kobe²

2:45pm - 5:10pm

External Resource:  Presentation



MS-66-1201-004_b.pdf

4:10pm - 4:30pm

Structural studies of Cysteine Synthase Complex obtained from *Klebsiella pneumoniae*.

Shubham Semwal¹, Deepansh Mody², Vibha Gupta², Julie Bouckaert¹

¹Unité de Glycobiologie Structurale et Fonctionnelle, UMR 8576, CNRS, 50 Avenue Halley, 59650 Villeneuve d'Ascq, France;

²Biotechnology Department, Jaypee Institute of Information Technology (JIIT), A-10, sector-62 NOIDA, 201309, India;
shubham.semwal@univ-lille.fr

External Resource:  Presentation



MS-66-730-005_b.pdf

4:30pm - 4:50pm

Crystal structure of a complex between the electron-transfer partners arsenite oxidase and cytochrome c552, from the arsenite respiring bacterium *Rhizobium* sp. NT-26.

Nilakhi Poddar¹, Joanne M Santini², Megan J Maher^{1,3}

¹School of Chemistry and The Bio21 Institute Molecular Sciences and Biotechnology Institute, The University of Melbourne, Parkville, 3052, Australia; ²Institute of Structural and Molecular Biology, Division of Biosciences, University College London, London WC1E 6BT, United Kingdom; ³Department of Biochemistry and Genetics, La Trobe Institute for Molecular Science, La Trobe University, Melbourne, Australia

External Resource:  Presentation



MS-66-1331-006_b.pdf

4:50pm - 5:10pm

Structural evidence for active site complementation and diverse oligomerization in two bacterial α -L-Fucosidases from the same organism

Jan Dohnálek¹, Terézia Kovařová^{1,2}, Tomáš Koval¹, Jan Stránský¹, Petr Kolenko¹, Jarmila Dušková¹, Patricie Vodičková², Vojtěch Spiwok², Eva Benešová², Petra Lipovová²

¹Institute of Biotechnology of the Czech Academy of Sciences, 25250 Vestec, Czech Republic; ²University of Chemistry and Technology, 166 28 Prague, Czech Republic

External Resource:  Presentation



MS-66-1268-007_b.pdf

MS-67: Crystallization mechanisms of small molecule systems

Location: **Terrace 2B**

Session Chair: **Duane Choquesillo-Lazarte**

Invited: **Ian Rosbottom (UK), Aurora Cruz-Cabeza (UK)**

Introduction

2:45pm - 2:50pm

Introduction to session

Duane Choquesillo-Lazarte



MS-67-1798-001.pdf

2:50pm - 3:20pm

CAN MOLECULAR FLEXIBILITY CONTROL CRYSTALLISATION?

Aurora Cruz-Cabeza

University of Manchester, Manchester, United Kingdom; aurora.cruzcabaza@manchester.ac.uk

External Resource:  Presentation



MS-67-1327-002_b.pdf

3:20pm - 3:50pm

Molecular, Solid-State and Surface Structures of the Conformational Polymorphic Forms of Ritonavir in Relation to their Physicochemical Properties

Ian Rosbottom

School of Chemical and Process Engineering, University of Leeds, LS2 9JT; irosbottom210289@gmail.com

2:45pm - 5:10pm

External Resource:



MS-67-1581-003_b.pdf

3:50pm - 4:10pm

Bridging the nucleation step – the link of molecular interactions in dilute solutions and the crystal structure

Katharina Edkins

University of Manchester, Manchester, United Kingdom; katharina.edkins@manchester.ac.uk

External Resource:



MS-67-827-004_b.pdf

4:10pm - 4:30pm

Controlling polymorphism of pharmaceutical cocrystals via polymer assisted cocrystallization in continuous processes

Anna Magdalena Golkowska, Marta Maria Kozakiewicz, Karol Przemysław Nartowski

Department of Drug Forms Technology, Wrocław Medical University, Wrocław, Poland; anna.golkowska@student.umed.wroc.pl

External Resource:



MS-67-940-005_b.pdf

4:30pm - 4:50pm

Crystallization of anionic small molecules with the help of a cation screen

Ekaterina Slyshkina, Jaclyn Parris, Bernhard Spingler

University of Zurich, Zurich, Switzerland; spingler@chem.uzh.ch

External Resource:



MS-67-919-006_b.pdf

4:50pm - 5:10pm

The Future of Co-crystallisation: A New Workflow Based on AI Predictions, the Crystal16 Platform and Electron Diffraction

Danny Stam^{1,2}, Carmen Guguta¹, Arianna Lanza², Gustavo Santiso-Quinones², Gunther Steinfeld², Doriana Ungur³, Coca Iordache³, Mihaela Pop³

¹Technobis Crystallization Systems B.V., Alkmaar, The Netherlands; ²ELDICO Scientific AG, 5234 Villigen, Switzerland; ³TeraCrystal, Cluj Napoca, Romania; ddpwtam@gmail.com

External Resource:



MS-67-780-007_b.pdf

MS-68: Symmetry aspects of magnetic order and magnetic properties

Location: **Club B**

Session Chair: **Mois Ilia Aroyo**

Session Chair: **Margarida Henriques**

Invited: **Laura Chaix (France), Fabio Orlandi (UK)**

Introduction

2:45pm - 2:50pm

Introduction to session

Mois Ilia Aroyo, Margarida Henriques



MS-68-1799-001.pdf

2:50pm - 3:20pm

Ba₃NbFe₃Si₂O₁₄:a model system to study magnetic chirality

LAURA CHAIX, RAFIK BALLOU, VIRGINIE SIMONET

Univ. Grenoble Alpes, CNRS, Grenoble INP, Institut Néel, 38000 Grenoble, France; laura.chaix@neel.cnrs.fr

External Resource:



MS-68-1022-002_b.pdf

2:45pm - 5:10pm

3:20pm - 3:50pm

Peculiar commensurate spin density wave in CeAuSb₂ under uniaxial stress



Fabio Orlandi¹, Richard Waite^{1,2}, Dmitry Sokolov³, Raquel A. Ribeiro⁴, Paul C. Canfield⁴, Pascal Manuel¹, Dmitry D. Khalyavin¹, Clifford W. Hicks⁴, Stephen M. Hayden²

¹ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, OX11 0QX, United Kingdom; ²H. H. Wills Physics Laboratory, University of Bristol, Bristol, BS8 1TL, United Kingdom; ³Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Straße 40, 01187 Dresden, Germany; ⁴Ames Laboratory, U.S. DOE, and Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, United States; fabio.orlandi@stfc.ac.uk

External Resource:



MS-68-1175-003_b.pdf

3:50pm - 4:10pm

Absolute sign of the Dzyaloshinskii-Moriya interaction in weak ferromagnets disclosed by polarized neutron diffraction



Henrik Friedrich Thoma^{1,2}, Vladimir Hutanu^{1,2}, Georg Roth², Manuel Angst³

¹Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH, 85748 Garching, Germany; ²Institute of Crystallography, RWTH Aachen University, 52056 Aachen, Germany; ³Jülich Centre for Neutron Science JCNS and Peter Grünberg Institut PGI, JARA-FIT, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany; h.thoma@fz-juelich.de

External Resource:



MS-68-851-004_b.pdf

4:10pm - 4:30pm

Resonant x-ray scattering of magnetic anisotropy and orbital ordering in Ca₂RuO₄



Dan Porter

Diamond Light Source Ltd, Didcot, United Kingdom; dan.porter@diamond.ac.uk

External Resource:



MS-68-216-005_b.pdf

4:30pm - 4:50pm

Low-temperature magnetic state of Ho₇Rh₃ studied by neutron diffraction and ac magnetic susceptibility



Artem Vaulin¹, Nikolay Baranov^{1,2}, Alexander Prekul¹, Takanori Tsutaoka³, Andey Gubkin^{1,2}

¹M.N. Mikheev Institute of Metal Physics of the Ural Branch of the Russian Academy of Sciences, Ekaterinburg, Russian Federation; ²UrFU them. the first President of Russia B.N. Yeltsin, Yekaterinburg, Russian Federation; ³Graduate School of Education, Hiroshima University, Higashi-Hiroshima, Japan; artavaulin@gmail.com

External Resource:



MS-68-715-006_b.pdf

MS-69a: Complex crystal structures - chemical crystallography



2:45pm - 5:10pm

Location: **Club A**

Session Chair: **Marie Colmont**

Session Chair: **Sergey V. Krivovichev**

Introduction

2:45pm - 2:50pm

Introduction to session



Marie Colmont, **Sergei Krivovichev**



MS-69a-1800-001.pdf

2:50pm - 3:15pm

Tellurides with monovalent Ga and In – from chains to networks



Tobias Lindemann¹, **Anna Isaeva**², **Oliver Oeckler**¹

¹Leipzig University, Leipzig, Germany; ²University of Amsterdam, Amsterdam, Netherlands; oliver.oeckler@gmx.de

External Resource:



MS-69a-803-002_b.pdf

3:15pm - 3:40pm



Elucidation and quantification of the factors underlying bond-length variation in inorganic solids for the design of non-oxide materials with superior functional properties

Olivier C. Gagné¹, Frank C. Hawthorne², Robert M. Hazen¹

¹Geophysical Laboratory, Carnegie Institution for Science, 5251 Broad Branch Rd. NW, Washington D.C., 20015 USA; ²Department of Geological Sciences, University of Manitoba, 125 Dysart Rd, Winnipeg, MB, Canada; ogagne@carnegiescience.edu

External Resource:



MS-69a-512-003_b.pdf

3:40pm - 4:05pm

Synthesis and investigation of the 4H and newly discovered 6H perovskite polymorphs of BaRhO₃ between 7 – 22 GPa.

Sean Dusan Injac¹, Yuanhui Xu^{1,2}, Fabio Denis Romero^{1,3}, Yuichi Shimakawa¹

¹Institute for Chemical Research, Kyoto University, Kyoto, Japan; ²Key Laboratory of Applied Chemistry, School of Environmental and Chemical Engineering, Yanshan University, Qinhuangdao, P.R. China; ³Hakubi Center for Advanced Research, Kyoto University, Kyoto, Japan; injac.seandusanalexander.6z@kyoto-u.ac.jp

External Resource:



MS-69a-734-004_b.pdf

4:05pm - 4:30pm

Enhancing the Chemical Flexibility of Hybrid Perovskites by Introducing Divalent Ligands

Paul J. Saines¹, Lydia G. Burley¹, James Beecham-Lonsdale¹, Anant Kumar Srivastava^{1,2}, Ines E. Collings³

¹School of Physical Sciences, University of Kent, Canterbury, Kent, United Kingdom; ²Department of Materials Engineering, Indian Institute of Science (IISc), Bangalore, Karnataka, India; ³Centre for X-ray Analytics, Empa – Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland; P.Saines@kent.ac.uk

External Resource:



MS-69a-791-005_b.pdf

4:30pm - 4:55pm

Temperature dependent structural studies of incommensurately modulated Rb₂ZnCl₄

Surya Rohith Kolla¹, Achim Mathias Schaller¹, Toms Rekis¹, Sitaram Ramakrishnan¹, Jin-Ke Bao¹, Leila Noohinejad², Sander Van Smaalen¹, Geoffroy de Laitre³, Marc de Boissieu³

¹Laboratory of Crystallography, University of Bayreuth, 95447 Bayreuth, Germany; ²DESY, Notkestrasse 85, 22607 Hamburg, Germany; ³Univ. Grenoble Alpes, CNRS, Grenoble INP, BP 75, 38402 Saint Martin d'Hères Cedex, France; Surya.Kolla@uni-bayreuth.de

External Resource:



MS-69a-442-006_b.pdf

MS-70: Matter at extreme conditions at SR and XFEL: complementarity of spectroscopy and diffraction

Location: **Club C**

Session Chair: **Angelika Dorothea Rosa**

Session Chair: **Ulf Zastrau**

Invited: **Virginia Monteseuro (Spain, ESRF), Emma McBride (USA, SLAC)**

Introduction

2:45pm - 2:50pm

Introduction to session

Angelika Dorothea Rosa, Ulf Zastrau



MS-70-1801-001.pdf

2:50pm - 3:20pm

Unveiling the structural and electronic interplay in 3d and 4f/5d compounds at high-pressure

Virginia Monteseuro¹, Juan Ángel Sans², Vera Cuartero³, Javier Ruiz-Fuertes¹, Catalin Popescu⁴, Fernando Rodríguez¹

¹DCITIMAC, Facultad de Ciencias, University of Cantabria, Spain; ²Universitat Politècnica de València, Spain; ³Centro Universitario de la Defensa de Zaragoza, Spain; ⁴ALBA-CELLS, Barcelona, Spain; virginia.monteseuro@unican.es

External Resource:



MS-70-1098-002_b.pdf

2:45pm - 5:10pm

3:20pm - 3:50pm

Phase Transition Lowering and Melting in Dynamically-Compressed Silicon and Germanium at the LCLS

Emma Elizabeth McBride

SLAC National Accelerator Laboratory, Menlo Park, United States of America; emcbride@slac.stanford.edu

External Resource:



MS-70-1352-003_b.pdf

3:50pm - 4:05pm

A new internally heated diamond anvil cell system for time resolved optical and x-ray measurements.

Yimin Mijiti^{1,2}, Marco Perri¹, Jean Coquet², Lucie Nataf², Marco Minicucci¹, Angela Trapananti¹, Tetsuo Irifune³, Francois Baudalet², Andrea Di Cicco¹

¹Physics Division, School of Science and Technology, University of Camerino, Via Madonna delle Carceri 9, Camerino (MC), 62032, Italy.; ²Synchrotron SOLEIL, L'Orme des Merisiers, Saint-Aubin, BP 48, 91192, Gif-sur-Yvette Cedex, France; ³Geodynamic Research Center, Ehime University, Matsuyama 790-8577, Japan.; emin.mijiti@unicam.it

External Resource:



MS-70-1154-004_b.pdf

4:05pm - 4:20pm

EMA beamline status and its XRD prospects

Guilherme A. Calligaris, Marcos A. S. Eleotério, José C. Corsaletti Filho, Hugo H. V. L. Campos, Joel A. V. Mendonça, Carlos Doro, Audrey D. Grockowiak, Ulisses F. Kaneko, Ricardo D. dos Reis, Narcizo M. Souza-Neto

Brazilian Synchrotron Light Laboratory (LNLS - CNPEM), Campinas, Brazil; guilherme.calligaris@lnls.br

External Resource:



MS-70-795-005_b.pdf

4:20pm - 4:35pm

Fast EXAFS measurement in piezo-driven single-crystal monochromatization scheme

Andrey Protsenko^{1,2}, Alexander Blagov^{1,2}, Anton Targonsky^{1,2}, Yan Eliovich^{1,2}, Alexander Rogachev², Sergey Yakunin², Michail Kovalchuk^{1,2}

¹FSRC "Crystallography & photonics" RAS; ²NRC "Kurchatov institute", Moscow, Russian Federation; 8xenderx8@gmail.com

External Resource:



MS-70-490-006_b.pdf

4:35pm - 4:50pm

Unveiling the Structural Behavior under Pressure of Filled $M_{0.5}Co_4Sb_{12}$ (M = K, Sr, La, Ce, and Yb) Thermoelectric Skutterudites

Joao Elias FIGUEIREDO SOARES RODRIGUES¹, Javier Gainza², Federico Serrano-Sánchez², Mateus Ferrer³, Catalin Popescu⁴, José Alonso²

¹ESRF, Grenoble, France; ²ICMM-Madrid, Spain; ³UFPEL, Brazil; ⁴ALBA, Spain; rodrigues.joaodelias@esrf.fr

External Resource:



MS-70-1155-007_b.pdf

4:50pm - 5:05pm

Towards higher densities of matter: ultra-high pre-compression in shock dynamic experiments

Anand Prashant Dwivedi¹, Sylvain Pettigirard², Karen Appel¹, Erik Brambrink¹, Zuzana Konôpková¹, Marius Millot³, Thomas Preston¹, Alessandra Ravasio⁴, Cornelius Strohm⁵, Ulf Zastrau¹, Valerio Cerantola¹

¹European X-ray Free Electron Laser facility GmbH; ²ETH-Zürich; ³Lawrence Livermore National Laboratory; ⁴Laboratoire pour l'Utilisation des Lasers Intenses, École Polytechnique; ⁵Deutsches Elektronen-Synchrotron DESY; anand.dwivedi@xfel.eu

External Resource:



MS-70-1289-008_b.pdf

2:45pm - 5:10pm

MS-71a: Disordered materials: spectroscopic and scattering techniques I

Location: **Terrace 2A**

Session Chair: **Simon Billinge**

Session Chair: **Angela Trapananti**

Invited: **Takeshi Egami (USA), Shinya Hosokawa (Japan)**

2:45pm - 2:50pm

Introduction to session

Simon Billinge, Angela Trapananti



MS-71a-1802-001.pdf

2:50pm - 3:20pm

What does the structure of liquid mean?

Takeshi Egami^{1,2}

¹University of Tennessee, Knoxville, United States of America; ²Oak Ridge National Laboratory, Oak Ridge, United States of America; egami@utk.edu

External Resource:



MS-71a-752-002_b.pdf

3:20pm - 3:50pm

Hyper-ordered structures and glass-forming abilities of Pd-based metallic glasses

Shinya Hosokawa

Kumamoto University, Kumamoto, Japan; shhosokawa@kumamoto-u.ac.jp

External Resource:



MS-71a-771-003_b.pdf

3:50pm - 4:10pm

Introducing the Pair-Angle Distribution Function: many-atom statistics of crystals and disordered materials

Andrew V. Martin¹, Jack Binns¹, Patrick Adams¹, Tamar L. Greaves¹, Connie Darmanin²

¹MIT University, Melbourne, Australia; ²ARC Centre of Excellence for Advanced Molecular Imaging, La Trobe Institute for Molecular Science, La Trobe University, Melbourne, Victoria, 3086, Australia.; andrew.martin@mit.edu.au

External Resource:



MS-71a-1086-004_b.pdf

4:10pm - 4:30pm

Group 13 precursor structures and their effect on oxide nanocrystal formation

Ida Gjerlevsen Nielsen, Sanna Sommer, Bo Brummerstedt Iversen

Center for Materials Crystallography, Department of Chemistry and iNano, Aarhus University, Aarhus C, Denmark; idani@chem.au.dk

External Resource:



MS-71a-576-005_b.pdf

4:30pm - 4:50pm

Extracting local symmetry of liquid metals from extended x-ray absorption fine structure using deep neural network

Fabio Iesari¹, Hiroyuki Setoyama², Toshihiro Okajima¹

¹Aichi Synchrotron Radiation Center (Seto, Aichi, Japan); ²Kyushu Synchrotron Light Research Center (Tosu, Saga, Japan); fabio.iesari@aichsr.jp

External Resource:



MS-71a-1027-006_b.pdf

4:50pm - 5:10pm

Disorder and dynamics of free and caged molecules in crystals

Guanqun Cai¹, Franz Demmel², Richard Dixey¹, Bernet E. Meijer¹, Shurong Yuan¹, Helen C. Walker², Anthony E. Phillips¹

¹Queen Mary University of London, London, United Kingdom; ²ISIS Neutron and Muon Source, Rutherford Appleton Laboratory, Harwell Oxford OX11 0QX, United Kingdom; a.e.phillips@qmul.ac.uk

External Resource:



MS-71a-1102-007_b.pdf

MS-72: New methods and strategies in NMR crystallography - in Honour of Francis Taulelle



Location: 223-4

Session Chair: **Martin Dracinsky**

Session Chair: **David Bryce**

Invited: **Sharon Ashbrook (UK)**, **Lyndon Emsley (Switzerland)**

Introduction

2:45pm - 2:50pm

Introduction to session

David Bryce, **Martin Dračinský**



MS-72-1803-001.pdf

2:50pm - 3:20pm

Investigating disorder in $A_2B_2O_7$ ceramics for waste encapsulation using NMR crystallography

Sharon E Ashbrook

University of St Andrews, St Andrews, United Kingdom; sema@st-andrews.ac.uk

External Resource:



MS-72-1012-002_b.pdf

3:20pm - 3:50pm

Structure determination of amorphous molecular solids by NMR crystallography

Lyndon Emsley

EPFL, Lausanne, Switzerland; lyndon.emsley@epfl.ch

External Resource:



MS-72-1171-003_b.pdf

3:50pm - 4:05pm

Anionic (dis)order and fluoride dynamics in complex transition metal oxyfluorides from NMR crystallography

Kent J. Griffith, **Kenneth R. Poeppelmeier**

Northwestern University, Evanston, United States of America; kent.griffith@northwestern.edu

External Resource:



MS-72-760-004_b.pdf

4:05pm - 4:20pm

NMR crystallography with microED

Yusuke Nishiyama^{1,2}

¹RIKEN-JEOL Collaboration Center; ²JEOL RESONANCE Inc.; yunishiy@jeol.co.jp

External Resource:



MS-72-1105-005_b.pdf

4:20pm - 4:35pm

NMR-Assisted Crystallography: Imaging Active Site Chemistry with Protons

Len Mueller

University of California - Riverside, Riverside, California, United States of America; leonard.mueller@ucr.edu

External Resource:



MS-72-1035-006_b.pdf

4:35pm - 4:50pm

NMR assisted structure determination of coordination polymers

Brijith Thomas^{1,3}, **Boyce S. Chang**^{2,3}, **Martin Thuo**^{2,3}, **Aaron Rossini**^{1,3}

¹Department of Chemistry, Iowa State University, Ames, IA 50010 USA; ²Department of Materials Science and Engineering, Iowa State University, Ames, IA 50011 USA; ³US DOE Ames Laboratory, Ames, Iowa, 50011, USA; brijith.ta@gmail.com

External Resource:





MS-72-1038-007_b.pdf

4:50pm - 5:05pm

A Strategy for Determining the Atomic-Resolution Structure of Micro-/Nanocrystalline Composite Solids

Jiri Brus

Institute of Macromolecular Chemistry CAS, Prague, Czech Republic; brus@imc.cas.cz

External Resource:



MS-72-1071-008_b.pdf

5:05pm - 5:20pm

A new NMR crystallographic protocol based on quadrupolar nuclei

Austin A. Peach^{1,2}, Kirill Levin³, Carl Fleischer^{1,2}, Sean T. Holmes^{1,2}, Robert Schurko^{1,2}

¹Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL, 32306; ²National High Magnetic Field Laboratory, Tallahassee, FL, 32310; ³Department of Chemistry and Biochemistry, University of Windsor, Windsor, ON, Canada N9B3P4; rschurko@fsu.edu

External Resource:



MS-72-1148-009_b.pdf

SF-5: Software Fayre 5

Location: 221-2

Session Chair: Martin Lutz

Session Chair: Claudia Millán

<http://www.cryst.chem.uu.nl/lutz/>

2:55pm - 3:40pm

Scipion-ed for electron crystallography

Viktor E. G. Bengtsson

Stockholm University, Stockholm, Sweden; viktor.bengtsson@mmk.su.se

External Resource:



3:40pm - 4:25pm

ConPlot: web-based tool for the visualization of protein contact maps and distograms integrated with other data

Filomeno Sanchez Rodriguez

University of Liverpool, Liverpool, United Kingdom; filomeno.sanchez-rodriguez@liverpool.ac.uk

4:25pm - 5:10pm

Topological analysis with ToposPro and TopCryst

Vladislav A. Blatov

Samara State Technical University, Samara, Russian Federation; blatov@topospro.com

External Resource:



5:10pm - 5:55pm

DISCUS Diffuse Scattering and Structure Simulation

Thomas Proffen¹, Reinhard Neder²

¹Oak Ridge National Laboratory, Oak Ridge, United States of America; ²Institute of Condensed Matter Physics, FAU Erlangen-Nürnberg; tproffen@ornl.gov

External Resource:



2:55pm - 5:55pm

5:10pm - 6:10pm

Afternoon break 5: Poster session C1, coffee/tea

Location: Exhibition and poster area

5:10pm - 6:10pm

Poster - 33 Chemical: Chemical crystallography

Poster session abstracts

Radomír Kužel



Poster - 33 Chemical-1960-001.pdf

Structure-activity relationship of imidazo[4,-f]1,10-phenanthroline type ligands and their Rhenium(I) complexes-photoluminescence and DNA intercalation

Lucy Ellen Kapp, Marietjie Schutte-Smith, Hendrik Gideon Visser

External Resource:



Poster - 33 Chemical-432-002_b.pdf

X-ray crystallography investigation of Iron-nucleotide ternary coordination complexes

Apurba Kumar Pal, Munirathinam Nethaji

Indian Institute Of Science, Bangalore, India; apurbapal@iisc.ac.in

External Resource:



Poster - 33 Chemical-1589-003_b.pdf

Exploring Structural Implications of diphosphinamine ligands in Medicine and Catalysis

Dumisani Kama¹, Alice Brink¹, Roger Alberto², Andreas Roodt¹

¹University of the Free State; ²University of Zürich; tomkama112@gmail.com

External Resource: <https://77>



Poster - 33 Chemical-879-004_b.pdf

Thermos-responsive single-component organic materials: Iso-symmetric phase transition, polymorphism and negative thermal expansion

SANJAY DUTTA, Parthapratim Munshi

SHIV NADAR UNIVERSITY, Dadri, India; sd669@snu.edu.in

External Resource:



Poster - 33 Chemical-520-005_b.pdf

Harnessing molecular rotations in plastic crystals: a holistic view for crystal engineering of adaptive soft materials

SUSOBHAN DAS, AMIT MONDAL, C MALLA REDDY

IISER Kolkata, Mohanpur, India; dassusobhan.chem@gmail.com

External Resource:



Poster - 33 Chemical-690-006_b.pdf

New insights about chemical etching for revelation of spontaneous fission tracks in garnets

Diogo Gabriel Sperandio¹, Cristiane Heredia Gomes², João Pedro de J. Santana³, Almiro Sant'Anna Junior⁴

¹Geology Department, Geosciences Institute, Federal University of Minas Gerais - UFMG, Belo Horizonte, MG, Brazil.; ²Federal University of Pampa – Unipampa, Caçapava do Sul, RS, Brazil.; ³Department of Geology, Federal University of Rio Grande do Sul – UFRGS.; ⁴Department of Mining Engineering, School of Mines, Federal University of Ouro Preto – UFOP, Ouro Preto, MG, Brazil; dsperandio@ufmg.br



Poster - 33 Chemical-357-007_b.pdf

Experimental Electron Density of Melamine

Emilie Skytte Vosegaard¹, Maja Krüger Thomsen¹, Mohammad Aref Hasen Mamakhel¹, Lennard Krause¹, Seiya Takahashi², Eiji Nishibori², Bo Brummerstedt Iversen¹

¹Department of Chemistry and Interdisciplinary Nanoscience Center (iNANO), Aarhus University, Aarhus, Denmark; ²Department of Physics, Faculty of Pure and Applied Sciences and Tsukuba Research Center for Energy Materials Science (TREMS), University of Tsukuba, Tsukuba, Ibaraki 305-8571, Japan; emilieskytte@chem.au.dk

External Resource:



Poster - 33 Chemical-1555-008_b.pdf

Resolving P-stereogenic enantiomers at nonambient-conditions

Tamás Holczbauer^{1,2}, Bence Varga³, Réka Herbay³, György Székely^{4,5}, János Madarász⁶, Béla Mátravölgyi³, Elemér Fogassy³, György Keglevich³, Péter Bagi³

¹Centre for Structural Science, Research Centre for Natural Sciences, Hungary; ²Institute of Organic Chemistry, Research Centre for Natural Sciences, Hungary; ³Department of Organic Chemistry and Technology, Budapest University of Technology and Economics,

Hungary; ⁴Advanced Membranes and Porous Materials Center, Physical Science and Engineering Division (PSE), King Abdullah University of Science and Technology (KAUST) Thuwal, 23955–6900, Saudi Arabia; ⁵Department of Chemical Engineering and Analytical Science, The University of Manchester, United Kingdom; ⁶Department of Inorganic and Analytical Chemistry Budapest University of Technology and Economics, Hungary; holczbauer.tamas@ttk.hu

External Resource:  Presentation



Poster - 33 Chemical-1548-009_b.pdf

HoF(OH)₂: A fluoride-containing holmium(III) hydroxide with UCl₃-type crystal structure

Felix C. Goerigk, Thomas Schleid

University of Stuttgart, Stuttgart, Germany; schleid@iac.uni-stuttgart.de

External Resource:  Presentation



Poster - 33 Chemical-1458-010_b.pdf

Crystallochemistry of Ni(II) complexes based on halogen derivatives of 8-hydroxyquinoline with different bridging of central atoms

Martin Russin¹, Erika Samoľová², Miroslava Litecká³, Ivan Potočník¹

¹Department of Inorganic Chemistry, Faculty of Science, Pavol Jozef Šafárik University in Košice, Slovakia; ²Department of Structure Analysis, Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic; ³Centre of Instrumental Techniques, Institute of Inorganic Chemistry, Czech Academy of Sciences, Řež, Czech Republic; martin.russin@student.upjs.sk

External Resource:  Presentation



Poster - 33 Chemical-1449-011_b.pdf

Zinc complexes with nitroderivatives of quinolin-8-ol

Michaela Harmošová¹, Erika Samoľová², Natália Kuncová¹, Ivan Potočník¹

¹Department of Inorganic Chemistry, Institute of Chemistry, P. J. Šafárik University in Košice, Moyzesova 11, 040 01 Košice, Slovakia; ²Institute of Physics of the Czech Academy of Sciences, Na Slovance 2, 182 21 Prague, Czech Republic; michaela.krescankova@student.upjs.sk

External Resource:  Presentation



Poster - 33 Chemical-1451-012_b.pdf

Radiation decay of (ZnI₂)₃(tpt)₂ crystal sponge

Václav Eigner

Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic; eigner@fzu.cz

External Resource:  Presentation



Poster - 33 Chemical-1484-013_b.pdf

Pr_{1.333}[P₂Se₆]: A link between two non-isotypic relatives

Beate M. Schulz, Pia Lena Lange, Thomas Schleid

University of Stuttgart, Stuttgart, Germany; pia.lange@iac.uni-stuttgart.de

External Resource:  Presentation



Poster - 33 Chemical-1430-014_b.pdf

Synthesis, characterization and *in vitro* activities of aniline dithiocarbamate crystals

Ayodele Temidayo Odularu

University of Fort Hare, Alice, South Africa; 201106223@ufh.ac.za

External Resource:  Presentation



Poster - 33 Chemical-994-015_b.pdf

Crystal structure of lead dinickel iron tris(orthophosphate): PbNi₂Fe(PO₄)₃

Said Ouatta, Elhassan Benhsina, Jamal Khmias, Abderrazzak Assani, Mohamed Saadi, Lahcen El Ammari

External Resource:



Poster - 33 Chemical-423-016_b.pdf

Butterfly Effect: Tracing Shape Memory Effect and Elastic Bending in a Conformationally Flexible Organic Salt

Avantika Hasija¹, S. R. N. Kiran Mangalampalli², Deepak Chopra¹

¹Indian Institute of Science Education and Research, Bhopal, Bhopal, India; ²SRM Institute of Science and Technology, Chennai, India; avantika16@iiserb.ac.in

External Resource:



Poster - 33 Chemical-744-017_b.pdf

Nucleophile assisted carbon dioxide fixation for a cleaner environment

Shaun Redgard, Andreas Roodt

University of The Free State, Bloemfontein, South Africa; shaunredgard@icloud.com

External Resource:



Poster - 33 Chemical-249-018_b.pdf

Structure diversity of transition metal coordination compounds based on pyridine derivative co-ligands

Merrill Margaret Wicht

Cape Peninsula University of Technology, Cape Town, South Africa; wichtm@cput.ac.za

External Resource:



Poster - 33 Chemical-387-019_b.pdf

Molecular packing of mesogenic bicyclohexylnitrile compounds

Sakuntala Gupta

Raiganj University, Raiganj, India; sakuntala_gupta@yahoo.com

External Resource:



Poster - 33 Chemical-735-020_b.pdf

Three differently-colored polymorphs of a diketopirrolpyrrole derivative having butyl groups

Tenma Muroya¹, Naoya Okada¹, Akehiro Toda², Kengo Imai², Toshinari Sekine², Shinya Matsumoto¹

¹Yokohama National University, Yokohama, Japan; ²Tokyo Printing Ink Mfg. Co., Ltd., Saitama, Japan; muroya-tenma-vc@ynu.jp

External Resource:



Poster - 33 Chemical-1475-021_b.pdf

Metastable disordered phase in flash-frozen Prussian Blue Analogues

Yevheniia Kholina, Arkadiy Simonov

ETH Zurich, Zurich, Switzerland; yevheniia.kholina@mat.ethz.ch

External Resource:



Poster - 33 Chemical-1559-022_b.pdf

RHODIUM (I) N,O HYDROXAMIC ACID COMPLEXES AS MODEL CATALYSTS

Mokete Motente, Johan Venter, Alice Brink

University of the Free State, Bloemfontein, South Africa; mokete.motente@gmail.com

External Resource:





Poster - 33 Chemical-1646-023_b.pdf

Syntheses and crystal structures of new ruthenium(II) organometallic compounds with NSAID type ligands

Martin Schoeller, Jan Moncol

Slovak University of Technology, Bratislava, Slovak Republic; martin.schoeller@stuba.sk

External Resource: Presentation



Poster - 33 Chemical-1690-025_b.pdf

Synthesis, phase characterization and crystal structure comparison of a self-made SmF_2 - SmFCl - SmFO mixture by XRD and EDX

Constantin Buyer, Thomas Schleid

University of Stuttgart, Stuttgart, Germany; constantin.buyer@jac.uni-stuttgart.de

External Resource: Presentation



Poster - 33 Chemical-1381-026_b.pdf

Polyoxometalate crystals exhibiting twinning by merohedry

Tomoji Ozeki

Nihon University, Tokyo, Japan; ozeki@chs.nihon-u.ac.jp

External Resource: Presentation



Poster - 33 Chemical-1387-027_b.pdf

Predicting molecular isomerism of symmetrical and unsymmetrical N,N' -diphenyl formamidines in the solid-state: crystal structure, Hirshfeld surface analysis, pairwise interaction energy, ΔH_{fusion} and ΔS_{fusion} determination

Sizwe Joshua Zamisa¹, Unathi Bongoza¹, Bernard Omondi²

¹School of Chemistry and Physics, University of KwaZulu Natal, Private Bag X54001, Durban, 4000, South Africa; ²School of Chemistry and Physics, University of KwaZulu Natal, Private Bag X01, Pietermaritzburg, South Africa; zamisas@ukzn.ac.za

External Resource: Presentation



Poster - 33 Chemical-1858-028_b.pdf

From neutral to salt cocrystal development to gain superior performance of NSAIDs

Ilma Nugrahani¹, Hidehiro Uekusa², Ayano Horikawa², Felicia Fisandra¹, Rizka A. Kumalasari¹, Winni N. Auli¹

¹Bandung Institute of Technology, Bandung, Indonesia; ²Department of Chemistry, School of Science, Tokyo Institute of Technology, Japan; ilma_nugrahani@yahoo.com

External Resource: Presentation



Poster - 33 Chemical-1919-029.pdf

Hirshfeld Atom Refinement of crystal structure and Hirshfeld surface analysis of five copper(II) fenamate complexes with N,N -diethylnicotinamide.

Milan Piroš, Jozef Švorec, Jan Moncol

Slovak University of Technology, Bratislava, Slovak Republic; jan.moncol@stuba.sk



Poster - 33 Chemical-1922-030_b.pdf

Poster - 34 Catalysis: Catalysis

Session Chair: **Valérie Briois**

Session Chair: **Andreas Roodt**



5:10pm - 6:10pm

Poster session abstracts

Radomír Kužel



Poster - 34 Catalysis-1961-001.pdf

In-situ XRPD analysis of active carbon supported Co-Mo ammonia synthesis catalysts activation

Agnieszka Wojciechowska, Paweł Adamski, Aleksander Albrecht, Artur Jurkowski

West Pomeranian University of Technology in Szczecin, ul. Pułaskiego 10, Szczecin, Poland; awojciechowska152@wp.zut.edu.pl

External Resource:



Poster - 34 Catalysis-1547-002_b.pdf

Dependence of wustite based iron catalyst crystallite size on ammonia synthesis reaction analysed by in-situ XRPD

Artur Jurkowski, Paweł Adamski, Aleksander Albrecht, Agnieszka Wojciechowska, Zofia Lendzion-Bieluń

West Pomeranian University of Technology in Szczecin, ul. Pułaskiego 10, Szczecin, Poland; artur.jurkowski@zut.edu.pl

External Resource:



Poster - 34 Catalysis-1545-003_b.pdf

How does precipitation pH affect structural transformations during activation of Co-Mo catalyst? In situ XRPD study

Aleksander Albrecht, Paweł Adamski, Mariena Nadziejko, Dariusz Moszyński

West Pomeranian University of Technology in Szczecin, Pułaskiego 10, 70-322 Szczecin, Poland; aleksander.albrecht@zut.edu.pl

External Resource:



Poster - 34 Catalysis-1544-004_b.pdf

In-situ XRPD study of ammonolysis of cobalt-molybdenum ammonia synthesis catalysts with defined Co to Mo ratio

Paweł Adamski, Aleksander Albrecht, Dariusz Moszyński

West Pomeranian University of Technology in Szczecin, ul. Pułaskiego 10, Szczecin, Poland; adamski_pawel@zut.edu.pl

External Resource:



Poster - 34 Catalysis-1543-005_b.pdf

Immobilization of tungsten trioxide on the surface of mesoporous silica: structural investigation of the role of crystalline water on photocatalyst stability.

Oussama Oulhakem

Materials Nano-Materials Unit, Energy Research Center, Mohammed V University in Rabat, Morocco;

oussama.oulhakem@um5s.net.ma

External Resource:



Poster - 34 Catalysis-565-006_b.pdf

Detailed information about the core/shell/surface structure of palladium nanoparticles by combined *in situ* and *operando* X-ray absorption and diffraction data

Aram Bugaev^{1,2}, Oleg Usoltsev¹, Alina Skorynina¹, Alexander Guda¹, Kirill Lomachenko³, Alexander Soldatov¹

¹Southern Federal University, Rostov-on-Don, Russia; ²Southern Scientific Center, Russian Academy of Science, Rostov-on-Don, Russia; ³European Synchrotron Radiation Facility, Grenoble, France; alinaskorynina@gmail.com

External Resource:



Poster - 34 Catalysis-539-007_b.pdf

Evolution of Pd/CeO₂ surface morphology in situ monitored by FTIR spectroscopy

Andrei Tereshchenko, Alexander Guda, Vladimir Polyakov, Yuri Rusalev, Alexander Soldatov

The Smart Materials Research Institute, Southern Federal University, 344090 Rostov-on-Don, Russia; tereshch1@gmail.com

External Resource:





Poster - 34 Catalysis-483-008_b.pdf

Crystal growth and structural studies of spinel ferrites

Jonas Ruby Sandemann, Bo Brummerstedt Iversen

Department of Chemistry & Interdisciplinary Nanoscience Center (iNANO), Aarhus University, Denmark; jonas@inano.au.dk

External Resource:



Poster - 34 Catalysis-1562-009_b.pdf

Poster - 35 Modulated: Composite and Incommensurate Modulated Crystals

Session Chair: **Sander van Smaalen**

Session Chair: **Sylvain Ravy**



5:10pm - 6:10pm

Poster session abstracts

Radomír Kužel



Poster - 35 Modulated-1962-001.pdf

A novel, statistical approach for structure determination of modulated pathogenesis-related protein (Hyp-1) complex with ANS

Joanna Maria Smietanska¹, Joanna Sliwiak², Mariusz Jaskolski², Mirosław Gilski², Zbigniew Dauter³, Ireneusz Buganski¹, Radosław Strzalka¹, Janusz Wolny¹

¹AGH University of Science and Technology, Krakow, Poland; ²Center for Biocrystallographic Research, Institute of Bioorganic Chemistry, Polish Academy of Sciences, Poznan, Poland; ³Synchrotron Radiation Research Section, MCL, National Cancer Institute, Argonne National Laboratory, Argonne IL 60439, USA; joanna.smietanska@fis.agh.edu.pl

External Resource:



Poster - 35 Modulated-1406-002_b.pdf

Incommensurately modulated structure - a means for increased luminescence efficiency in the solid state

Anna Maria Makal

University of Warsaw, Warszawa, Poland; amakal@chem.uw.edu.pl

External Resource:



Poster - 35 Modulated-1242-003_b.pdf

Successive transitions to modulated states in the {R}Pt₂Si₂ family

Elen Duverger-Nédellec^{1,2}, Michał Falkowski^{2,3,4}, Petr Doležal², Volodymyr Buturlim², Alexander Andreev³, Jérémy Forté⁵, Lise-Marie Chamoreau⁵, Ladislav Havela²

¹Institut de Chimie de la Matière Condensée de Bordeaux, Pessac cedex, France; ²Charles University, Department of Condensed Matter Physics, Prague, Czech Republic; ³Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic; ⁴Institute of Molecular Physics, Polish Academy of Sciences, Poznań, Poland; ⁵Institut Parisien de Chimie Moléculaire, Sorbonne Université, Paris, France; elenduvergernedellec@gmail.com

External Resource:



Poster - 35 Modulated-936-004_b.pdf

Local analysis of periodically modulated quasi-one-dimensional structures

Marion Antonia van Midden¹, Herman J. P. van Midden¹, Craig Bennett², Albert Prodan¹, Erik Zupanič¹

¹Jožef Stefan Institute, Ljubljana, Slovenia; ²Dept. of Physics, Acadia University, Wolfville, Nova Scotia, Canada; marion.van.midden@ijs.si

External Resource:



Poster - 35 Modulated-306-005_b.pdf

Dynamical Properties of the Incommensurately Modulated Rb₂ZnCl₄ Phase

Geoffroy de Laitre¹, Surya Rohith Kotla², Sander Van Smaalen², Yvan Sidis³, Quentin Berrod^{3,4}, Jean-Marc Zanotti^{3,4}, Jacques Ollivier⁴, Stéphane Raymond^{4,5}, Frédéric Bourdarot^{4,5}, Andrea Piovano⁴, Christine Opagiste⁶, Stéphane

Coindeau^{1,7}, Marc de Boissieu¹

¹Laboratoire de Science et Ingénierie des Matériaux et Procédés, CNRS, Université Grenoble Alpes, Grenoble INP, 38402 Saint Martin d'Hères, France.; ²Laboratory of Crystallography, University of Bayreuth, 95447 Bayreuth, Germany.; ³Laboratoire Léon Brillouin (CEA-CNRS), Université Paris-Saclay CEA Saclay, 91191 Gif-sur-Yvette, France.; ⁴Institut Laue-Langevin, CS 20156, 38000 Grenoble, France.; ⁵CEA Grenoble, IRIG, MEM, NRS, Université Grenoble Alpes, 38000 Grenoble, France.; ⁶Institut Neel, CNRS, Université Grenoble Alpes, Grenoble INP, 38000 Grenoble, France.; ⁷CMTC, Grenoble INP, CNRS, 38402 Saint-Martin d'Hères, France.; Geoffroy.de-Laitre@simap.grenoble-inp.fr

External Resource:



Poster - 35 Modulated-731-006_b.pdf

High-temperature structural studies of d-AlCuRh – phasonic stabilization

Radosław Strzalka, Ireneusz Bugański, Janusz Wolny

AGH University of Science and Technology, Krakow, Poland; strzalka@fis.agh.edu.pl

External Resource:



Poster - 35 Modulated-1028-007_b.pdf

Dodecahedral Structures from D₆ lattice

Nazife Ozdes Koca

Sultan Qaboos University, Muscat, Oman; nazife@squ.edu.om

External Resource:



Poster - 35 Modulated-629-008_b.pdf

Modulated molecular crystals: Incommensurate, high Z' forms and their variation as function of temperature and stress

Somnath Dey¹, Debasish Halder², Chilla Malla Reddy², Andreas Schönleber³, Sander van Smaalen³

¹Institute of Crystallography, RWTH Aachen University, Jägerstraße 17-19, 52066 Aachen, Germany; ²Department of Chemical Sciences, Indian Institute of Science Education and Research (IISER) Kolkata, Mohanpur 741246, India; ³Laboratory of Crystallography, University of Bayreuth, D-95440 Bayreuth, Germany; somnathdey226@gmail.com

External Resource:



Poster - 35 Modulated-309-009_b.pdf

Crystal symmetry for incommensurate helical and cycloidal modulations

Piotr Fabrykiewicz, Radosław Przeniosło, Izabela Sosnowska

Faculty of Physics, University of Warsaw, Pasteura 5 PL 02-093 Warsaw, Poland; Piotr.Fabrykiewicz@fuw.edu.pl

External Resource:



Poster - 35 Modulated-1425-010_b.pdf

Exploration of new quasicrystals and approximants by using machine learning

Hirotaka Uryu¹, Tsunetomo Yamada¹, Hiroyuki Takakura², Yuki Inada³, Kaoru Kimura³, Ryuji Tamura¹, Chang Liu⁴, Ryo Yoshida⁴

¹Tokyo University of Science; ²Hokkaido University; ³The University of Tokyo; ⁴The Institute of Statistical Mathematics; 1521512@ed.tus.ac.jp

External Resource:



Poster - 35 Modulated-1578-011_b.pdf

Poster - 36 Disordered: Disordered materials

Session Chair: **Simon Billinge**

Session Chair: **Angela Trapananti**



5:10pm - 6:10pm

Poster session abstracts

Radomir Kužel



Poster - 36 Disordered-1963-001.pdf

Preferred orientation in modified clay/polymer composite films

Patricia Carolina Rivas Rojas¹, Vera Alejandra Alvarez², Cristian Huck Iriart¹

¹Laboratory of Applied Crystallography, School of Science and Technology, National University of San Martin, San Martin, Buenos Aires CP B1650, Argentina; ²CoMP, INTEMA, National University of Mar del Plata, Mar del Plata CP 7600, Argentina; privasr@unsam.edu.ar

External Resource:



Poster - 36 Disordered-534-002_b.pdf

Surface sensitive x-ray spectroscopy (TREXS) for nanoscale surface study and multi-modal development

Hitoshi Abe^{1,2,3}, Yasuhiro Niwa¹, Masao Kimura^{1,2}

¹High Energy Accelerator High Energy Accelerator Research Organization (KEK), Tsukuba, Japan; ²SOKENDAI (The Graduate University for Advanced Studies)Tsukuba, Japan; ³Ibaraki University, Mito, Japan; hitoshi.abe@kek.jp

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Poster - 36 Disordered-594-003_b.pdf

Structural refinement of aqueous zirconium oxychloride using total scattering methods

Joe Andrew Rawlinson, Jennifer Elizabeth Readman

University of Central Lancashire, Preston, United Kingdom; JRawlinson@uclan.ac.uk

External Resource:



Poster - 36 Disordered-613-004_b.pdf

Disordering mechanism during Li-ion intercalation in nano-rutile TiO₂

Christian K. Christensen¹, Ananya R. Balakrishna², Bo B. Ierssen³, Yet-Ming Chiang², Dorte B. Ravnsbæk¹

¹University of Southern Denmark, Odense S, Denmark; ²Massachusetts Institute of Technology, Cambridge, MA, USA; ³Aarhus University, Aarhus, Denmark; christiankc@sdu.dk

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Poster - 36 Disordered-958-005_b.pdf

An anomalous diffraction study of Cu₂Zn(Ge,Si)Se₄

Daniel M. Töbrens, Galina Gurieva, Sara Niedenzu, Götz Schuck, Susan Schorr

Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany; daniel.toebbens@helmholtz-berlin.de

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Poster - 36 Disordered-848-006_b.pdf

Spectroscopic and Pair Distribution Evidence for Hexamethylenetetramine (HMT) as Adsorbents and Absorbents of Nano-ceria

Jonathan Campbell Hanson¹, Milinda Abeykoon¹, Dimitriy Vovchok¹, Siu Wai Chan²

¹Brookhaven National Laboratory, Upton, NY, United States of America; ²Columbia University, New York, NY, United States of America; hanson1@bnl.gov

External Resource:



Poster - 36 Disordered-949-007_b.pdf

The structure of bulk Al₂O₃ glass

Shinji Kohara¹, Yohei Onodera^{2,1}, Shuta Tahara³, Hideki Hashimoto⁴, Hidetaka Asoh⁴

¹National Institute for Materials Science, Tsukuba, Japan; ²Kyoto University, Kumatori, Japa; ³University of Ryukyus, Nishihara, Japan; ⁴Kogakuin University, Hachioji, Japan; KOHARA.Shinji@nims.go.jp

External Resource:





Poster - 36 Disordered-745-008_b.pdf

Structure of sustainable lead-free low-melting vanadate glass

Yohei Onodera^{1,2}, Shinji Kohara², Takuya Aoyagi³, Takashi Naito³, Jens R. Stellhorn⁴, Shinya Hosokawa⁵, Hiroo Tajiri⁶, Alex C. Hannon⁷, László Pusztai⁸, Pál Jóvári⁸

¹Kyoto University, Osaka, Japan; ²National Institute for Materials Science, Ibaraki, Japan; ³Hitachi Ltd., Ibaraki, Japan; ⁴Hiroshima University, Hiroshima, Japan; ⁵Kumamoto University, Kumamoto, Japan; ⁶Japan Synchrotron Radiation Research Institute, Hyogo, Japan; ⁷Rutherford Appleton Laboratory, Oxon, UK; ⁸Wigner Research Centre for Physics, Budapest, Hungary; y-onodera@rri.kyoto-u.ac.jp

External Resource: Presentation



Poster - 36 Disordered-805-009_b.pdf

Poster - 37 Biomineralization: Biomineralization, advanced biomimetic materials



5:10pm - 6:10pm

Session Chair: **Giuseppe Falini**

Session Chair: **Juan Manuel Garcia-Ruiz**

Poster session abstracts

Radomír Kužel



Poster - 37 Biomineralization-1964-001.pdf

Ecomorphological, behavioural and physiological patterns in otoliths

Quinzia Palazzo^{1,6}, Marco Stagioni², Steven Raaijmakers³, Robert G. Belleman³, Fiorella Prada^{4,6}, Simona Fermani¹, Jörg U. Hammel⁵, Jaap Kaandorp³, Stefano Goffredo^{4,6}, **Giuseppe Falini**^{1,6}

¹Department of Chemistry <<Giacomo Ciamician>>, University of Bologna, Via Selmi 2, 40126 Bologna, Italy; ²Laboratory of Fisheries and Marine Biology at Fano, Department of Biological, Geological and Environmental Sciences, University of Bologna, Viale Adriatico 1/N, 61032, Fano, Italy; ³Computational Science Lab, University of Amsterdam, Science Park 904, 1098XH, Amsterdam, the Netherlands; ⁴Marine Science Group, Department of Biological, Geological and Environmental Sciences, University of Bologna, Via Selmi 3, 40126 Bologna, Italy; ⁵Institute of Materials Physics, Helmholtz-Zentrum Geesthacht, Max-Planck-Straße 1, Geesthacht, D-21502, Germany; ⁶Fano Marine Center, The Inter-Institute Center for Research on Marine Biodiversity, Resources and Biotechnologies, Viale Adriatico 1/N 61032 Fano, Italy; giuseppe.falini@unibo.it

External Resource: Presentation



Poster - 37 Biomineralization-1455-002_b.pdf

Rietveld and pair-distribution function analysis of nanogranular mesocrystalline shells of hyaline foraminifers

Anthea I. Arns^{1,2,3}, Ralf Schiebel¹, David Evans², Lothar Fink³, Edith Alig³, Martin U. Schmidt³, Jolien Linckens², Anne Jantschke⁴, Gerald H. Haug^{1,5}

¹Department of Climate Geochemistry, Max Planck Institute for Chemistry, Hahn-Meitner-Weg 1, 55128 Mainz, Germany; ²Institute of Geosciences, Goethe University Frankfurt, Altenhöferallee 1, 60438 Frankfurt a.M., Germany; ³Institute of Inorganic and Analytical Chemistry, Goethe University Frankfurt, Max-von-Laue-Str. 7, 60438 Frankfurt a.M., Germany; ⁴Institute of Geosciences, Johannes Gutenberg University Mainz, Johann-Joachim-Becher-Weg 21, 55128 Mainz, Germany; ⁵Department of Earth Sciences, ETH Zurich, Sonneggstrasse 5, 8092 Zurich, Switzerland; anthea.arns@mpic.de

External Resource: Presentation



Poster - 37 Biomineralization-1303-003_b.pdf

Bio-complexes as supermolecules: towards the design of idealized peptide-based ligands

Joanna Bojarska

Technical University of Lodz, Poland, Lodz, Poland; joanna.bojarska@p.lodz.pl



Poster - 37 Biomineralization-1651-004_b.pdf

Unique Mode(s) of Action of Ions on Calcium Oxalate Mineralization

Bryan Genciano Alamani

University of the Philippines Diliman, Quezon City, Philippines; bgalamani@up.edu.ph

External Resource: Presentation



Poster - 37 Biomineralization-1652-005_b.pdf

Antimicrobial nanolayered and nanofibrous metal phosphates for prospective biomedical applications

Alaa Adawy¹, Zakariae Amghouz², Camino Trobajo³, Jose R. Garcia³

¹Unit of Electron Microscopy and Nanotechnology, Institute for Scientific and Technological Resources (SCTs), University of Oviedo, 33006 Oviedo, Spain; ²Department of Material Science and Metallurgical Engineering, University of Oviedo, 33203 Gijón, Spain; ³Department of Organic and Inorganic Chemistry, University of Oviedo, 33006 Oviedo, Spain; Hassanalaa@uniovi.es

External Resource:



Poster - 37 Biomineralization-1657-006_b.pdf



Poster - 37 Biomineralization-1657-006_c.pdf

Biomimetic Strategies for 4.0 V All-Solid-State Flexible Supercapacitor: Moving toward Eco-friendly, Safe, Aesthetic, and High-Performance Devices

Wei-Tsung Chuang

National Synchrotron Radiation Research Center, Hsinchu, Taiwan; weitsung@nsrc.org.tw

External Resource:



Poster - 37 Biomineralization-1731-007_b.pdf

Crystal structure and SOD activity of a hybrid lysozyme including an amino acid Schiff base copper complex

Tetsundo Furuya¹, Natsuki Katsuumi¹, Kenichi Kitanishi¹, Masaki Unno², Takashiro Akitsu¹

¹Department of Chemistry, Faculty of Science, Tokyo University of Science, 1-3 Kagurazaka, Shinjuku-ku, Tokyo 162-8601, Japan; ²Graduate School of Science and Engineering, Ibaraki University, Hitachi, Ibaraki 316-8511, Japan; 1319610@ed.tus.ac.jp

External Resource:



Poster - 37 Biomineralization-1889-008_b.pdf

Poster - 38 Energy: Materials for energy conversion and storage

Session Chair: **Stefan Adams**

Session Chair: **Jean-Marc Joubert**



5:10pm - 6:10pm

Poster session abstracts

Radomír Kužel



Poster - 38 Energy-1965-001.pdf

Hydrogen bonding in hybrid organic-inorganic perovskite materials

Xiaoping Wang

Oak Ridge National Laboratory, Oak Ridge, United States of America; wangx@ornl.gov

External Resource:



Poster - 38 Energy-610-002_b.pdf

Combined crystallochemical and quantum-chemical search for new high-valent chalcogen-containing ionic conductors

Yelizaveta Morkhova^{1,2}, Artem Kabanov^{1,2}, Tillman Leisegang^{2,3}, Manuel Rothenberger³, Vladislav Blatov^{1,2}

¹Samara Center for Theoretical Materials Science, Samara, Russian Federation; ²Samara Center for Theoretical Materials Science, Samara Polytech, Samara, Russian Federation; ³IEP TUBAF, Freiberg, Germany; elizimofeeva@mail.ru

External Resource:



Poster - 38 Energy-264-003_b.pdf

Cation disorder in zinc-group IV- nitride and oxide nitride semiconductor materials revealed through neutron diffraction

Susan Schorr^{1,2}, Joachim Breternitz^{1,3}, Zhenyu Wang^{1,2}

¹Helmholtz-Zentrum Berlin fuer Materialien und Energie, Berlin, Germany; ²Freie Universitaet Berlin, Institute of Geological Sciences, Berlin, Germany; ³Universitaet Potsdam, Institute of Chemistry, Potsdam, Germany; susan.schorr@helmholtz-berlin.de

External Resource:



Poster - 38 Energy-922-004_b.pdf

Crystal structure and Mössbauer studies of gallium iron borate single crystals

Igor Lyubutin¹, Nikita Snegirev¹, Ekaterina Smirnova¹, Sergey Starchikov¹, Marianna Lyubutina¹, Vladimir Artemov¹, Sergey Yagupov², Mark Strugatsky², Yuliya Mogilenec², Olga Alekseeva¹

¹Shubnikov Institute of Crystallography of FSRC "Crystallography and Photonics" RAS, 119333, Moscow, Russia; ²Physics and Technology Institute, V.I. Vernadsky Crimean Federal University, 295007, Simferopol, Russia; lyubutinig@mail.ru

External Resource:  Presentation



Poster - 38 Energy-625-005_b.pdf

Model construction of actuation performance of a photo-bending crystal using machine learning-based regression.

Kazuki Ishizaki¹, Yuki Hagiwara¹, Hideko Koshima², Takuya Taniguchi³, Toru Asahi^{1,2}

¹Graduate School of Advanced Science and Engineering, Waseda University, Tokyo, Japan; ²Research Organization for Nano & Life Innovation, Waseda University, Tokyo, Japan; ³Center for Data Science, Waseda University, Tokyo, Japan; kazuki.143@toki.waseda.jp

External Resource:  Presentation



Poster - 38 Energy-1265-006_b.pdf

Expanded chemistry and mixed ionic-electronic conductivity in vanadium-substituted variants of γ -Ba₄Nb₂O₉

Alex Brown¹, Bettina Schwaighofer^{2,3}, Max Avdeev^{1,4}, Bernt Johannessen⁵, Ivana Radosavljevic Evans², Chris Ling¹

¹School of Chemistry, The University of Sydney, Sydney, Australia; ²Department of Chemistry, Durham University, Science Site, South Road, Durham DH1 3LE, U.K.; ³Institut Laue Langevin, 71 Rue de Martyrs, 38000 Grenoble, France; ⁴Australian Nuclear Science and Technology Organisation, Lucas Heights NSW 2234, Australia; ⁵Australian Synchrotron, Clayton, Victoria, 3168 Australia; alexander.brown@sydney.edu.au

External Resource:  Presentation



Poster - 38 Energy-838-007_b.pdf

Environmentally Friendly Rhodium(I) Model Catalysts tailored by various bidentate and monodentate (water-soluble) ligand.

Zanele Morerwa, Alice Brink, Andreas Roodt

University of The Free State, Pretoria, South Africa; z.morerwa@gmail.com

External Resource:  Presentation



Poster - 38 Energy-481-008_b.pdf

Synthesis, characterization of high-temperature properties and evaluation of REBa₂Cu₃O_{6+δ} (RE = La, Nd and Y) as cathode for Intermediate Temperature Solid Oxide Fuel Cells.

Joaquín Grassi¹, Leopoldo Suescun¹, Mario Alberto Macías², Adriana Serquis³

¹Facultad de Química, Universidad de la República, Montevideo, Uruguay; ²Departamento de Química, Universidad de los Andes, Bogotá, Colombia; ³Departamento de Caracterización de Materiales, CAB-INN-CONICET-CNEA, Bariloche, Argentina; joaquingrassi@fq.edu.uy

External Resource:  Presentation



Poster - 38 Energy-535-009_b.pdf

Lattice disorder and oxygen migration pathways in pyrochlore and defect-fluorite oxides

Frederick Marlon¹, Zhaoming Zhang², Yaunpeng Zhang³, Thomas Proffen³, Chris Ling¹, Brendan Kennedy¹

¹School of Chemistry, The University of Sydney, Sydney; ²Australian Nuclear Science and Technology Organisation; ³Neutron Scattering Division, Oak Ridge National Laboratory; frederick.marlon@sydney.edu.au

External Resource:  Presentation



Poster - 38 Energy-761-010_b.pdf

LiFe_{2-x}In_xSbO₆ Oxides as Li-ion Cathode Materials

Xabier Martínez de Irujo Labalde¹, Josie-May Whitnear², Samuel Booth², Bonan Zhu³, Michael Hayward¹

¹Inorganic Chemistry Laboratory, University of Oxford, Oxford, United Kingdom; ²Department of Chemical and Biological Engineering, The University of Sheffield, United Kingdom; ³Department of Chemistry, University College London, United Kingdom; xabier.martinezdeirujolabalde@chem.ox.ac.uk

External Resource:



Poster - 38 Energy-1523-011_b.pdf

Enigmatic Structure Property Behaviour in SOFC & SOEC electrolyte materials

David Gordon Billing, Caren Billing, Mathias Kiefer, Sikhumbuzo Masina

University of the Witwatersrand, Johannesburg, South Africa; dave.billing@wits.ac.za

External Resource:



Poster - 38 Energy-1522-012_b.pdf

Time resolved structure analysis of vibrating gallium phosphate under alternating electric field

Shinobu Aoyagi¹, Kazuhira Miwa¹, Hitoshi Osawa², Kuniyisa Sugimoto^{2,3}, Hiroaki Takeda⁴

¹Department of Information and Basic Science, Nagoya City University, Nagoya 467-8501, Japan; ²Research and Utilization Division, Japan Synchrotron Radiation Research Institute, Sayo, Hyogo 679-5198, Japan; ³Institute for Integrated Cell-Material Sciences (iCeMS), Kyoto University, Yoshida-Ushinomiya-cho, Sakyo-ku, Kyoto 606-8501, Japan; ⁴Graduate School of Science and Engineering, Saitama University, 255 Shimo-Okubo, Sakura-ku, Saitama, 338-8570, Japan; aoyagi@nsc.nagoya-cu.ac.jp

External Resource:



Poster - 38 Energy-1579-013_b.pdf

Analysis of multi-layer thin film materials using benchtop XRD and XRF systems

Dr. Simon Welzmler¹, Eric Berthier², Raphael Yerly³

¹Thermo Fisher Scientific, Dreieich, Germany; ²Thermo Fisher Scientific, Artenay, France; ³Thermo Fisher Scientific, Dreieich, Germany; Raphael.Yerly@thermofisher.com



Poster - 38 Energy-1426-014_b.pdf

Exploring the magnetocaloric effect in the $Ln(HCO_2)(C_2O_4)$ family of Metal-Organic Frameworks

Mario Falsaperla¹, Gavin B.G. Stenning², Ivan da Silva², Paul J. Saines¹

¹School of Physical Sciences, University of Kent, Canterbury, UK; ²ISIS Facility, STFC Rutherford Appleton Laboratory, Didcot, UK; mf494@kent.ac.uk

External Resource:



Poster - 38 Energy-781-015_b.pdf

Operando SAXS/WAXS studies for structure determination of energy storage materials using a unique electrochemical-scattering cell

Heiner Santner¹, Christian Prehal², **Andreas Keilbach**¹, Georg Urstöger¹, Andrew Jones¹

¹Anton Paar GmbH, Graz, Austria; ²ETH Zürich, Zürich, Switzerland; andreas.keilbach@anton-paar.com

External Resource:



Poster - 38 Energy-1574-016_b.pdf

The role of Al^{3+} , Dy^{3+} co-doping on the structure-property correlations in NASICON-type $LiTi_2(PO_4)_3$ solid-state electrolytes

Gugulethu Charmaine Nkala^{1,2}, Sikhumbuzo Masina¹, Caren Billing¹, Roy Peter Forbes¹, David Gordon Billing^{1,2}

¹Molecular Sciences Institute, School of Chemistry, University of the Witwatersrand, Johannesburg, South Africa; ²DSI-NRF Centre of Excellence in Strong Materials (CoE-SM); 721270@students.wits.ac.za

External Resource:



Poster - 38 Energy-301-017_b.pdf

Poster - 39 Neutrons: Neutron scattering

Session Chair: **Esko Oksanen**

Session Chair: **Matthew Paul Blakeley**

Session Chair: **Jiri Kulda**

5:10pm - 6:10pm



Poster session abstracts

Radomir Kužel



Poster - 39 Neutrons-1966-001.pdf

Identification of crystallographic planes of a polyhedral crystal at SENJU

Akiko Nakao¹, **Taketo Moyoshi**¹, **Kentaro Moriyama**¹, **Takeshi Matsumura**², **Kenshirou Iba**², **Shigeo Ohara**³, **Yoshihisa Ishikawa**¹, **Koji Munakata**¹, **Takashi Ohhara**⁴, **Ryoji Kiyonagi**⁴

¹Neutron Science and Technology Center, CROSS, Tokai, Ibaraki 319-1106, Japan; ²Department of Quantum Matter, AdSM, Hiroshima University, Hiroshima 739-8530, Japan; ³Department of Physical Science and Engineering, Graduate School of Engineering, Nagoya Institute of Technology, Nagoya 466-8555, Japan; ⁴J-PARC Center, Japan Atomic Energy Agency, Tokai, Ibaraki 319-1195, Japan; a_nakao@cross.or.jp

External Resource: Presentation



Poster - 39 Neutrons-1470-002_b.pdf

Upgrades of a TOF single-crystal neutron diffractometer SENJU for improvement of versatility

Takashi Ohhara¹, **Ryoji Kiyonagi**¹, **Akiko Nakao**², **Koji Munakata**², **Yoshihisa Ishikawa**², **Kentaro Moriyama**², **Itaru Tamura**¹, **Koji Kaneko**¹

¹J-PARC Center, Japan Atomic Energy Agency, Tokai, Ibaraki, Japan; ²Neutron Science and Technology Center, Comprehensive Research Organization for Science and Society, Tokai, Ibaraki, Japan; takashi.ohhara@j-parc.jp

External Resource: Presentation



Poster - 39 Neutrons-1372-003_b.pdf

Macromolecular Neutron Diffraction at the Heinz Maier-Leibnitz Zentrum

Andreas Ostermann¹, **Tobias E. Schrader**²

¹Technical University Munich, Heinz Maier-Leibnitz Zentrum MLZ, Garching, Germany; ²Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Garching, Germany

External Resource: Presentation



Poster - 39 Neutrons-1441-004_b.pdf

Towards generalised diffraction integration software: neutron diffraction analysis in DIALS

David McDonagh¹, **David Waterman**^{1,2}

¹Science and Technology Facilities Council, Didcot, United Kingdom; ²CCP4, Research Complex at Harwell, Rutherford Appleton Laboratory, Didcot, United Kingdom; david.mcdonagh@stfc.ac.uk

External Resource: Presentation



Poster - 39 Neutrons-1593-005_b.pdf

Toward elucidating the mechanism of lytic polysaccharide monooxygenases: Chemical insights from X-ray and neutron crystallography

Gabriela C. Schröder^{1,2}, **Flora Meilleur**^{1,2}

¹Department of Molecular and Structural Biochemistry, North Carolina State University, Raleigh, NC 27695, USA; ²Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA.

External Resource: Presentation



Poster - 39 Neutrons-1617-006_b.pdf

Application of machine learning and kernel density estimation for efficient data treatment on single crystal diffraction data

Ryoji Kiyonagi¹, **Takashi Ohhara**¹, **Akiko Nakao**², **Koji Munakata**², **Yoshihisa Ishikawa**², **Kentaro Moriyama**²

¹J-PARC center, Japan Atomic Energy Agency, Ibaraki, Japan; ²Neutron Science and Technology center, Comprehensive Research Organization for Science and Society, Ibaraki, Japan; ryoji.kiyonagi@j-parc.jp

External Resource: Presentation



Poster - 39 Neutrons-1447-007_b.pdf

Protein neutron diffraction experiment with dynamic nuclear polarization

Ichiro Tanaka, Himeka Nishino, Hideki Yamauchi, Yohei Noda, Tomoki Maeda, Satoshi Koizumi
Ibaraki University, Ibaraki, Japan

External Resource:  Presentation



Poster - 39 Neutrons-1567-008_b.pdf

In search of anharmonic motion of H-atoms

Szymon Marcin Sutula¹, Maura Malinska¹, Laura Canadillas Delgado², Oscar Ramon Fabelo Rosa², Krzysztof Woźniak¹

¹Department of Chemistry, University of Warsaw, Pasteura 1, 02093 Warszawa, Poland; ²Institut Laue-Langevin, 71 Ave Des Martyrs, CS 20156, 38042, Grenoble Cedex 9, Grenoble, France; s.sutula@uw.edu.pl

External Resource:  Presentation



Poster - 39 Neutrons-444-009_b.pdf

Poster - 40 NMR: NMR crystallography

Session Chair: **David Bryce**

Session Chair: **Martin Dracinsky**



5:10pm - 6:10pm

Poster session abstracts

Radomír Kužel



Poster - 40 NMR-1967-001.pdf

Exploring zinc-terephthalate complexes through multi nuclear ssNMR and *in-situ* reaction monitoring by Raman spectroscopy

Cesar Leroy¹, Thomas-Xavier Métro², Danielle Laurencin¹

¹ICGM, Univ Montpellier, CNRS, ENSCM, Montpellier, France; ²IBMM, Univ Montpellier, CNRS, ENSCM, Montpellier, France; cesar.leroy@umontpellier.fr

External Resource:  Presentation



Poster - 40 NMR-1192-002_b.pdf

Solid - State NMR Crystallography Analysis of Lorlatinib, an Active Pharmaceutical Ingredient

Zainab Rehman

University of Warwick, Coventry, United Kingdom; zainab.rehman@warwick.ac.uk

External Resource:  Presentation



Poster - 40 NMR-1125-003_b.pdf

KN-25: A Crystallographic Snapshot of SARS-CoV-2 Main Protease Maturation Process and the Discovery of Inhibitors

Location: **Club A**

Session Chair: **Julie Bouckaert**

Glaucius Oliva



6:10pm - 7:00pm

A Crystallographic Snapshot of SARS-CoV-2 Main Protease Maturation Process

Gabriela D Noske¹, Aline Minali Nakamura¹, Victor O Gawriljuk¹, Rafaela S Fernandes¹, Gustavo M A Lima², Igor V D Rosa¹, Humberto D Pereira¹, Ana C M Zeri³, Andrey F Z Nascimento³, Marjorie C L C Freire¹, **Glaucius Oliva**¹, Andre S Godoy¹

¹Institute of Physics of Sao Carlos, University of Sao Paulo, Brazil; ²BioMAX, MAX IV Laboratory, Lund, Sweden; ³Brazilian Synchrotron Light Laboratory (LNLS), Campinas, Brazil; oliva@ifsc.usp.br

External Resource:  Presentation



KN-25-632-001_b.pdf

KN-26: Complexity in crystals and minerals

Location: **Terrace 2A**

Session Chair: **Milan Rieder**

Sergey Krivovichev



6:10pm - 7:00pm

Natural polyoxometalates: diversity, complexity and divergence from synthetic chemistry

Sergey V. Krivovichev^{1,2}

External Resource:  Presentation



KN-26-1566-001_b.pdf

6:10pm - 7:00pm **KN-27: The crystal and the rose: On the impact of crystals and crystallography in art and mind** (+)
 Location: **Terrace 2B**
 Session Chair: **Abel MORENO**
Juan Manuel Garcia-Ruiz

The crystal and the rose: On the impact of crystals and crystallography on arts and mind
Juan Manuel Garcia-Ruiz
 Laboratorio de Estudios Cristalográficos. Consejo Superior de Investigaciones Científicas-Universidad de Granada;
juanmanuel.garcia@csic.es

External Resource:  Presentation



KN-27-776-001_a.doc



KN-27-776-001_b.pdf

7:10pm - 7:50pm **PL-2: In situ and ex situ studies of battery materials with magnetic resonance and diffraction methods** (+)
 Location: **Terrace 2A**
 Session Chair: **Juergen Senker**
Clare Grey
Video

In situ and ex situ studies of battery materials with magnetic resonance and diffraction methods
Clare Grey
 University of Cambridge, Cambridge, United Kingdom; cpg27@cam.ac.uk

External Resource:  Presentation



PL-2-1915-001_b.pdf

7:50pm - 10:15pm **IUCr-3: IUCr assembly** (+)
 Location: **Club H**
 Session Chair: **Sven Lidin**
 Session Chair: **Luc Van Meervelt**
 Session Chair: **Alex Ashcroft**
 IUCr assembly 3
Videos: Part 1 - China bid - Australia - Election

Date: Friday, 20/Aug/2021

9:00am - 9:50am **KN-28: 4th generation SR and XFEL facilities: new era in crystallography and material science** (+)
 Location: **Terrace 2A**
 Session Chair: **Elena Boldyreva**
Aleksandr Blagov

Fourth-generation Synchrotron radiation and XFEL facilities: new era in crystallography and material science.
Alexander Eugenievich Blagov
 National Research Center «Kurchatov Institute», Moscow, Russian Federation; blagov_ae@mail.ru

External Resource:  Presentation



KN-28-1668-001_b.pdf

9:00am - 9:50am **KN-29: Crystal engineering of adaptive smart materials: from mechanical bending to self-healing** (+)
 Location: **Terrace 2B**
 Session Chair: **Masaki Kawano**
Malla Reddy

Crystal engineering of adaptive smart materials: from mechanical bending to self-healing
C Malla Reddy
 Indian Institute of Science Education and Research (IISER) Kolkata, Mohanpur, 741246, India; cmreddy@iiserkol.ac.in

External Resource:  Presentation



KN-29-1641-001_b.pdf

9:00am - 9:50am **KN-30: Structure guided inhibitor discovery targeting a membrane receptor involved in atherosclerosis** (+)

Location: **Club A**
Session Chair: **Julie Bouckaert**
Arockiasamy Arulandu

Structure guided inhibitor discovery targeting a membrane receptor involved in atherosclerosis

Arockiasamy Arulandu¹, Akanksha Tomar¹, Azeem Khan¹, Sibasis Sahoo¹, Muthu Sankar Aathi¹, Shobhan Kuila¹, Anmol Chande¹, Jawahar L Mehta², Kottayil I Varughese³

¹International Centre for Genetic Engineering and Biotechnology, New Delhi, India; ²University of Arkansas for Medical Sciences and the Central Arkansas Veterans Healthcare System, Little Rock, Arkansas, United States; ³University of Arkansas for Medical Sciences, Little Rock, Arkansas, United States.; sam@icgeb.res.in

External Resource:  Presentation



KN-30-1878-001_a.doc



KN-30-1878-001_b.pdf

9:50am - 10:20am

Morning break 6: Posters, coffee/tea

Location: **Exhibition and poster area**

MS-73: Machine learning in biological and structural sciences

Location: **Terrace 2B**

Session Chair: **Rita Giordano**

Session Chair: **Harold Roger Powell**

Invited: **Melanie Vollmar (UK), Sergei Grudinin (France)**

Introduction

10:20am - 10:25am

Introduction to session

Rita Giordano, Harold Roger Powell



MS-73-1804-001.pdf

10:20am - 12:45pm

10:25am - 10:55am

Predicting experimental phasing success for data triaging

Melanie Vollmar¹, Irakli Sikharulidze¹, Gwyndaf Evans^{1,2}

¹Diamond Light Source, Didcot, United Kingdom; ²Rosalind Franklin Institute, Didcot, United Kingdom

External Resource:  Presentation



MS-73-938-002_b.pdf

10:55am - 11:25am

Deep learning entering the post-protein structure prediction era : new horizons for structural biology

Sergei Grudinin

Univ. Grenoble Alpes, CNRS, Grenoble INP, LJK, 38000 Grenoble, France; sergei.grudinin@univ-grenoble-alpes.fr

External Resource:  Presentation



MS-73-1173-003_b.pdf

11:25am - 11:45am

How machine learning can supplement traditional quality indicators - and the human eye: A case study

Andrea Thörn¹, Kristopher Nolte¹, Yunyun Gao¹, Sabrina Stäb¹, Philip Kollmannsberger²

¹Universität Hamburg, Germany; ²Julius-Maximilians-Universität Würzburg, Germany

External Resource:  Presentation



MS-73-1196-004_b.pdf

11:45am - 12:05pm

Learning structure-energy relationships for the prediction of molecular crystal structures

Graeme M Day

University of Southampton, Southampton, United Kingdom

External Resource:  Presentation



MS-73-965-005_b.pdf

12:05pm - 12:25pm

New generalized crystallographic descriptors for structural machine learning

James Cumby, Sohan Seth, Ruizhi Zhang

External Resource:



MS-73-869-006_b.pdf

12:25pm - 12:45pm

Analysis of pre-edge XANES spectra of Fe:SiO₄ system by using machine learning methods.

Danil Pashkov, Alexander Guda, Sergey Guda, Alexander Soldatov

Southern Federal University, Rostov-on-Don, Russian Federation; pashkov@sfned.ru

External Resource:



MS-73-341-007_b.pdf

MS-74: Structural biology of receptors, signaling and membrane proteins

Location: **Club A**

Session Chair: **SUSAN KAY BUCHANAN**

Session Chair: **Michael Parker**

Invited: **Robert Keenan (USA)**, **Isabel Moraes (UK)**

Introduction

10:20am - 10:25am

Introduction to session

Susan Kay Buchanan, **Michael Parker**



MS-74-1805-001.pdf

10:25am - 10:55am

Structures of the archaerhodopsin-3 transporter reveal that disordering of internal water networks underpins receptor sensitization

Isabel Moraes¹, Peter J. Judge², Juan F. Bada Juarez², Danny Axford³, Tristan Kwan¹, Anthony Watts²

¹National Physical Laboratory, Teddington, TW11 0LW, UK; ²Biochemistry Department, University of Oxford, South Parks Road, Oxford, OX1 3QU, UK; ³Diamond Light Source, Harwell Science and Innovation Campus, Didcot, OX11 0DE, UK

External Resource:



MS-74-1004-002_b.pdf

10:55am - 11:25am

An ER translocon for multi-pass membrane protein biogenesis

Philip T McGilvray¹, S Andrei Anghel¹, Arunkumar Sundaram¹, Frank Zhong¹, Michael J Trnka², James R Fuller¹, Hong Hu¹, Alma L Burlingame², **Robert J Keenan¹**

¹University of Chicago, Chicago, United States of America; ²University of California, San Francisco, United States of America

External Resource:



MS-74-1383-003_b.pdf

11:25am - 11:45am

To eat or not to eat: Cryo-EM structure of melanocortin receptor 4 reveals mechanism of a "hunger switch" initiating satiety signaling.

Oksana Degtjarik¹, Hadar Israeli^{1,2}, Li F. Chan³, Danny Ben-Zvi², Masha Y. Niv⁴, Peter J. McCormick³, Moran Shalev-Benami¹

¹Department of Chemical and Structural Biology, Weizmann Institute of Science, Rehovot, Israel; ²Department of Developmental Biology and Cancer Research, The Hebrew University-Hadassah Medical School, Jerusalem, Israel; ³Centre for Endocrinology, William Harvey Research Institute, Barts and the London School of Medicine, Queen Mary, University of London, Charterhouse Square, London, UK; ⁴Faculty of Agriculture, The Hebrew University, Israel; degtjarik648@gmail.com

External Resource:



MS-74-1296-004_b.pdf

11:45am - 12:05pm

Unravelling the molecular architecture of the Commander assembly

Michael David Healy¹, Joanna Sacharz², Tristan Croll³, David A Stroud², Brett M Collins¹

¹The University of Queensland, Brisbane, Australia; ²University of Melbourne, Melbourne, Australia; ³Cambridge Institute for Medical Research, Cambridge, United Kingdom

External Resource:





MS-74-809-005_b.pdf

12:05pm - 12:25pm

Two-component pore formation by the novel CDCL proteins ALY short and ALY long from *Elizabethkingia anophelis*

Bronte A Johnstone¹, Sara L Lawrence², Michelle P Christie¹, Rodney K Tweten³, Craig J Morton¹, Michael W Parker^{1,2}

¹Department of Biochemistry and Molecular Biology, Bio21 Molecular Science and Biotechnology Institute, University of Melbourne, Parkville, VIC, 3010, Australia; ²ACRF Rational Drug Discovery Centre, St. Vincent's Institute of Medical Research, Fitzroy, VIC 3065, Australia; ³Department of Microbiology and Immunology, University of Oklahoma, Health Sciences Center, Oklahoma City, OK 73104, USA; bjohnstone@student.unimelb.edu.au

External Resource:



MS-74-466-006_b.pdf

12:25pm - 12:45pm

Mechanistic insights into the synergistic activation of the RXR–PXR heterodimer by endocrine disruptor mixtures

Vanessa Delfosse¹, Tiphaine Huet¹, Deborah Harrus¹, Meritxell Graneli¹, Maxime Bourguet², Caroline Gardia-Parège³, Barbara Chiavarina³, Marina Grimaldi³, Sébastien Le Mével⁴, Pauline Blanc¹, David Huang¹, Jakob Gruszczyk¹, Barbara Demeneix⁴, Sarah Cianférani², Jean-Baptiste Fini⁴, Patrick Balaguer³, William Bourguet¹

¹Center for Structural Biology, Montpellier, France; ²Laboratoire de Spectrométrie de Masse Bioorganique, Strasbourg, France; ³Institut de Recherche en Cancérologie, Montpellier, France; ⁴Muséum National d'Histoire Naturelle, Paris, France

External Resource:



MS-74-689-007_b.pdf

MS-75: Small- and Wide-Angle Scattering for industrial materials far from equilibrium

Location: **Club D**

Session Chair: **Jan Ilavsky**

Session Chair: **Semra IDE**

Invited: **Masato Ohnuma (Japan), Elliot Paul Gilbert (Australia)**

Introduction

10:20am - 10:25am

Introduction to session

Jan Ilavsky, Semra Ide



MS-75-1806-001.pdf

10:25am - 10:55am

Characterising Food Materials and the Case for Extended q Scattering

Elliot Paul Gilbert

ANSTO, NSW, Australia; elliott.gilbert@ansto.gov.au

External Resource:



MS-75-883-002_b.pdf

10:55am - 11:25am

"Slow operand" measurements by laboratory small-angle X-ray scattering

Masato Ohnuma¹, Shigeru Kuramoto², Isamu Kaneda³

¹Hokkaido University, Sapporo, Japan; ²Ibaraki University, Hitachi, Japan; ³Rakuno Gakuen University, Ebetsu, Japan; ohnuma.masato@eng.hokudai.ac.jp

External Resource:



MS-75-1170-003_b.pdf

11:25am - 11:45am

Breaking Bad: Towards Certifiable Additively Manufactured Alloys Using Post-Build Heat Treatment

Fan Zhang¹, Carelyn E. Campbell¹, Mark R. Stoudt¹, Lyle E. Levine¹, Andrew J. Allen¹, Eric A. Lass², Greta Lindwall³

¹Material Measurement Laboratory, National Institute of Standards and Technology, Gaithersburg, MD 20899, USA; ²Department of Materials Science and Engineering, University of Tennessee, Knoxville, TN 37996, USA; ³Department of Materials Science and Engineering, KTH Royal Institute of Technology, Brinellvägen 8, 114 28 Stockholm, Sweden; fan.zhang@nist.gov

External Resource:



10:20am - 12:45pm



MS-75-606-004_b.pdf

11:45am - 12:05pm

Time-evolution of Au and Ag nanofluids prepared by direct deposition of gas aggregated nanoparticles into the liquid polymer

Tereza Košutová¹, Daniil Nikitin², Pavel Pleskunov², Renata Taflichuk², Andrei Choukourov², Milan Dopita¹

¹Department of Condensed Matter Physics, Faculty of Mathematics and Physics, Charles University, Ke Karlovu 5, 121 16, Prague, Czech Republic; ²Department of Macromolecular Physics, Faculty of Mathematics and Physics, Charles University, V Holešovičkách 2, Prague, 180 00, Czech Republic; kosutovat@gmail.com

External Resource: Presentation



MS-75-1090-005_b.pdf

12:05pm - 12:25pm

XRD, USAXS, SAXS and WAXS Investigations of ferroelectric PZN-4.5PT nanoparticles thin Films

Rémi Ndioukane¹, Abdoul Kadri Diallo¹, Ndeye Coumba Yandé Fall¹, Moussa Touré¹, Diouma KOBOR¹, Tabbetha Amanda Dobbins², Jan Ilavsky³, Laurent Lebrun⁴

¹Laboratoire de Chimie et de Physique des Matériaux (LCPM), University Assane Seck of Ziguinchor (UASZ), Quartier Néma 2, BP 523, Ziguinchor, Senegal; ²Department of Physics & Astronomy, Provost Fellow (2019), Division of University Research, Rowan University, Oak Hall North 109, 201 Mullica Hill Road Glassboro, NJ 08028-1701; ³X-Ray Science Division, Advanced Photon Source, Argonne National Laboratory 9700 S. Cass Avenue, bldg 433A002, Lemont, IL 60439, USA; ⁴Univ Lyon, INSA-Lyon, LGEF, EA682 - 8 rue de la Physique, F-69621, Villeurbanne, France; dkobor@univ-zig.sn

External Resource: Presentation



MS-75-1166-006_b.pdf

12:25pm - 12:45pm

The nSoft Autonomous Formulation Laboratory: SANS/SAXS/WAXS Liquid Handling for Industrial Formulation Discovery

Peter A. Beaucage, Tyler B. Martin

National Institute of Standards and Technology, Gaithersburg, United States of America; peter.beaucage@nist.gov

External Resource: Presentation



MS-75-1165-007_b.pdf

MS-76(59b): Crystal chemistry with emerging technology II

Location: **Club C**

Session Chair: **Consiglia Tedesco**

Session Chair: **Toru Asahi**

Introduction

10:20am - 10:25am

Introduction to session

Consiglia Tedesco, Toru Asahi



MS-76(59b)-1807-001.pdf

10:25am - 10:55am

In situ study of chemical synthesis using high-energy X-ray diffraction on beamline I12 at Diamond Light Source

Oxana V. Magdysyuk, Thomas Connolley, Robert Atwood, Stefan Michalik

Diamond Light Source Ltd., Didcot, United Kingdom; Oxana.Magdysyuk@diamond.ac.uk

External Resource: Presentation



MS-76(59b)-860-002_b.pdf

10:55am - 11:25am

The solid-state chemistry of rhodium(I) pincer complexes under extreme conditions.

Alexandra Longcake, Jeremiah P. Tidey, Mark S. Senn, Adrian B. Chaplin

University of Warwick, Coventry, United Kingdom; alex.longcake@warwick.ac.uk

External Resource: Presentation

10:20am - 12:45pm



MS-76(59b)-336-003_b.pdf

11:25am - 11:45am

Insight into the Structural Variations of Fergusonite-Type Structures: Combined Experimental and Computational Studies

Bryce Mullens¹, Maxim Avdeev^{1,2}, Helen Brand³, Subrata Mondal⁴, Ganapathy Vaitheeswaran⁵, Brendan Kennedy¹

¹School of Chemistry, The University of Sydney, New South Wales 2006, Australia; ²Australian Nuclear Science and Technology Organisation, Lucas Heights, New South Wales 2234, Australia; ³Australian Synchrotron, 800 Blackburn Road, Clayton, Victoria 2168, Australia; ⁴Advanced Centre of Research in High Energy Materials (ACRHEM), University of Hyderabad, Prof. C. R. Rao Road, Gachibowli, Hyderabad 500 046, Telangana, India; ⁵School of Physics, University of Hyderabad, Prof. C. R. Rao Road, Gachibowli, Hyderabad 500 046, Telangana, India; bmul2806@uni.sydney.edu.au

External Resource:



MS-76(59b)-807-004_b.pdf

11:45am - 12:05pm

Growth and spectroscopic studies of Na₂W₂O₇ crystals doped with Ce⁺⁴ and Cr⁺³ ions, promising scintillation detectors of elementary particles

Veronika Grigorjeva, Mariana Rakhmanova, Alexey Ryadun

Nikolaev Institute of Inorganic Chemistry SB RAS, Novosibirsk, Russian Federation; grigorjeva@niic.nsc.ru

External Resource:



MS-76(59b)-896-005_b.pdf

12:05pm - 12:25pm

Correlation between structural studies and third order NLO properties of three new semi-organic compounds

Rim Benali-Cherif¹, Radhwane Takouachet¹, El-Eulmi Bendelf², Nourredine Benali-Cherif³

¹Abbes Laghrour Khenchela University, Khenchela, Algeria; ²Laboratoire de Cristallographie, Résonance Magnétique et Modélisations (CRM2, UMR CNRS 7036), France; ³Houari Boumediène (USTHB)-Member of Algerian Academy of Sciences and Technology (AAST) Algiers. Algeria; rym_46@hotmail.com

External Resource:



MS-76(59b)-268-006_b.pdf

12:25pm - 12:45pm

Structural, magnetic and optical properties study of tellurium-based: Sr_{3-x}Pb_xFe₂TeO₉ (0 ≤ x ≤ 2.25) double perovskites

Abdelhadi El Hachmi¹, Bouchaib Manoun^{1,2}, Mohammed Sajieddine³, Peter Lazor⁴

¹Laboratoire Rayonnement Matière et Instrumentation, S3M, FST, University Hassan 1er, 26000 Settat, Morocco; ²Materials Science and nano-engineering (MSN), University Mohammed VI Polytechnic, Lot 660 Hay Moulay Rachid, 43150 Ben Guerir, Morocco; ³Material Physics Laboratory, Faculty of Sciences and Techniques, Sultan Moulay Sliman University, B.P. 523, 23000 Beni-Mellal, Morocco; ⁴Department of Earth Sciences, Uppsala University, SE-752 36, Uppsala, Sweden; elhachmi.abdelhadi@gmail.com



MS-76(59b)-231-007_b.pdf

MS-77(71b): Disordered materials: spectroscopic and scattering techniques II

Location: 223-4

Session Chair: **Simon Billinge**

Session Chair: **Angela Trapananti**

Invited: **Lars G. M. Pettersson** (Sweden), **Maxwell Terban** (Germany)

Introduction

10:20am - 10:25am

Introduction to session

Simon Billinge, Angela Trapananti



MS-77(71b)-1808-001.pdf

10:25am - 10:55am

SpecSwap-RMC: A Generalized RMC Approach to Structure, Combining Scattering and Spectroscopic Data

Lars G.M. Pettersson

Stockholm University, Stockholm, Sweden; lgm@fysik.su.se

External Resource:



10:20am - 12:45pm



MS-77(71b)-1343-002_b.pdf

10:55am - 11:25am

Developing more precise structural descriptions of layered covalent organic frameworks using total scattering data

Maxwell W. Terban¹, Lars Grunenberg^{1,2}, Alexander M. Pütz^{1,2}, Sebastian Bette¹, Gökçen Savasci^{1,2,3}, Robert E. Dinnebier¹, Bettina V. Lotsch^{1,2,3}

¹Max Planck Institute for Solid State Research, Stuttgart, Germany; ²Department of Chemistry, Ludwig-Maximilians-Universität (LMU), Munich, Germany; ³Exzellenzcluster E-conversion, Garching, Germany and Center for NanoScience, Munich, Germany; m.terban@fkf.mpg.de

External Resource:



MS-77(71b)-1304-003_b.pdf

11:25am - 11:45am

Order-disorder transitions in battery electrodes studied by operando X-ray scattering

Dorthe Ravnsbæk, Christian Kollé Christensen, Christian Lund Jakobsen, Martin Karlsen

University of Southern Denmark, Odense M, Denmark; dora@sdu.dk

External Resource:



MS-77(71b)-954-004_b.pdf

11:45am - 12:05pm

Insight into the structure of SiO₂-supported Ni-Ga nanoparticles for catalytic application via X-ray absorption spectroscopy and total scattering

Nora K. Zimmerli, Paula M. Abdala, Christoph R. Mueller

ETH Zurich, Zurich, Switzerland; norazi@ethz.ch

External Resource:



MS-77(71b)-1164-005_b.pdf

12:05pm - 12:25pm

Tuneable Local Structure in Thermoelectric Crystals

Nikolaj Roth

University of Oxford, Oxford, United Kingdom; nikolajroth@gmail.com

External Resource:



MS-77(71b)-844-006_b.pdf

12:25pm - 12:45pm

Structure of complex aluminosilicate oxide-glasses: the role of zinc intermediate element.

Andrea Bernasconi^{1,2}, Monica Dapiaggi¹, Daniel T Bowron³, Giovanni Agostini^{2,4}, Alessandro Pavese⁵

¹University of Milan, Milano, Italy; ²ESRF The European Synchrotron, Grenoble, France; ³ISIS Pulsed Neutron and Muon Source, Didcot, UK; ⁴ALBA Synchrotron, Barcelona, Spain; ⁵University of Torino, Torino, Italy; andrea.bernasconi@hotmail.it

External Resource:



MS-77(71b)-814-007_b.pdf

MS-78: Science meets art: X-ray spectrometry and X-ray diffraction in art and archaeology

Location: **Club H**

Session Chair: **Gilberto Artioli**

Session Chair: **Sebastian Bette**

Invited: **Katrien Keune (Netherlands)**, **Christoph Berthold (Germany)**

Introduction

10:20am - 10:25am

Introduction to session

Gilberto Artioli, **Sebastian Bette**



MS-78-1809-001.pdf

10:20am - 12:45pm

10:25am - 10:55am

Operation Night Watch: macro- and microscale X-ray imaging studies on the Rembrandts' masterpiece *The Night Watch* in the Rijksmuseum.

Katrien Keune¹, Victor Gonzalez¹, Annelies Loon¹, Frederique Broers¹, Nouchka Keyser de¹, Petria Noble¹, Frederik VanMeert², Steven DeMeyer², Koen Janssens²

¹Rijksmuseum, Amsterdam, Netherlands, The; ²AXES Research Group, NANOLab Centre of Excellence, University of Antwerp, Belgium.; k.keune@rijksmuseum.nl

External Resource:



MS-78-1485-002_b.pdf

10:55am - 11:25am

X-ray Microdiffraction of Cultural Heritage: Potentials und Limitations

Christoph Berthold

University of Tuebingen, CCA-BW, Tübingen, Germany; christoph.berthold@uni-tuebingen.de

External Resource:



11:25am - 11:45am

XRPD as a tool for the study of pigment-binder interactions: from metal formates to long-chain carboxylates

Silvie Švarcová¹, Eva Kočí¹, Petr Bezdička¹, Silvia Garrappa¹, Jiří Plocek¹, Ruslan Barranikov¹, Libor Kobera²

¹Institute of Inorganic chemistry of the Czech Academy of Sciences, Husinec-Řež 1001, 250 68 Husinec-Řež, Czech Republic;

²Institute of Macromolecular Chemistry of the Czech Academy of Sciences, Heyrovského nám. 2, 162 06, Praha 6, Czech Republic;

svarcova@iic.cas.cz

External Resource:



MS-78-1045-004_b.pdf

11:45am - 12:05pm

Effects of soft tissue on the crystallographic changes to bone mineral upon heating

Hannah Louise Cross, Charlene Elizabeth Greenwood

Keele University, Liverpool, United Kingdom; h.l.cross@keele.ac.uk

External Resource:



MS-78-623-005_b.pdf

12:05pm - 12:25pm

A multidisciplinary study unveils the nature of a Roman ink of the I century AD

Chiaramaria Stani¹, Lara Gigli², Simone Pollastri², Mirta Sibilia³, Alessandro Migliori³, Francesco D'Amico², Chiara Schmid⁴, Sabina Lichen⁵, Matteo Crosera⁵, Gianpiro Adami⁵, Pierluigi Barbieri⁵, Jasper R. Plaisier², Giuliana Aquilanti², Lisa Vaccari², Stefano Buson⁶, Federica Gonzato⁶

¹CERIC-ERIC, Basovizza, Trieste, Italy; ²Elettra Sincrotrone Trieste S.C.p.A, Basovizza, Trieste, Italy; ³Nuclear Science and

Instrumentation Laboratory, Physics section, IAEA, Seibersdorf, Austria; ⁴Department of Engineering and Architecture, University of

Trieste, Trieste, Italy; ⁵Department of Chemical and Pharmaceutical Sciences, University of Trieste, Trieste, Italy; ⁶Museo Nazionale Atestino, Este, Padova, Italy; chiaramaria.stani@ceric-eric.eu

External Resource:



MS-78-789-006_b.pdf

12:25pm - 12:45pm

A new tool for ancient artefact conservation studies: Electron Diffraction Tomography to study blue corrosion product in Chinese Bronze sample

Partha Pratim Das¹, Enrico Mugnaioli², Quanyu Wang³, Stavros Nicolopoulos¹, Mauro Gemmi²

¹NanoMEGAS SPRL, Rue Émile Claus 49 bte 9, 1050, Brussels, Belgium; ²Center for Nanotechnology Innovation@NEST, Istituto Italiano di Tecnologia, Piazzale San Silvestro 12, 56127, Pisa, Italy; ³Institute of Cultural Heritage, Shandong University, 72 Jimo Binhailu, Qingdao 266237, China; partha@nanomegas.com

External Resource:



MS-78-841-007_b.pdf

MS-79(69b): Complex structures of minerals and inorganic materials

Location: **Club B**

Session Chair: **Marie Colmont**

Session Chair: **Sergey V. Krivovichev**

Introduction

10:20am - 12:45pm

10:20am - 10:25am

Introduction to session

Marie Colmont, Sergei Krivovichev



MS-79(69b)-1810-001.pdf

10:25am - 10:55am

Tracing electron density changes in langbeinite under pressure

Roman Gajda¹, Dongzhou Zhang², Jan Parafiniuk³, Przemysław Dera⁴, Krzysztof Woźniak¹

¹Biological and Chemical Research Centre, Department of Chemistry, University of Warsaw, 101 Żwirki i Wigury, Warszawa, 02-089, Poland; ²APS, University of Chicago, 9700 S Cass Ave, Bldg 434A, Argonne, IL 60439, USA; ³Institute of Geochemistry, Mineralogy and Petrology, Department of Geology, University of Warsaw, Żwirki i Wigury 93, Warszawa 02-089, Poland; ⁴Hawaii Institute of Geophysics and Planetology, School of Ocean and Earth Science and Technology, University of Hawaii at Manoa, 1680 East West Road, Honolulu, Hawaii 96822, USA; romanbg@chem.uw.edu.pl

External Resource: Presentation



MS-79(69b)-1185-002_b.pdf

10:55am - 11:25am

Experimental Electron Density Distribution and QTAIM Topological Analysis for the Perovskite Mineral: Sulphohalite – Na₆(SO₄)₂FCI

Agata Wróbel, Roman Gajda, Krzysztof Woźniak

Department of Chemistry, Biological and Chemical Research Centre, University of Warsaw, Poland.; am.wrobel2@student.uw.edu.pl

External Resource: Presentation



MS-79(69b)-1366-003_b.pdf

11:25am - 11:45am

Direct observation of pressure induced charge density redistribution at ions in zeolite, hsianghualite

Marcin Stachowicz, Roman Gajda, Krzysztof Woźniak

University of Warsaw, Warsaw, Poland; marcin.stachowicz@uw.edu.pl

External Resource: Presentation



MS-79(69b)-1310-004_b.pdf

11:45am - 12:05pm

Structural studies of titanium and zirconium silicate ion-exchange materials for the treatment of nuclear waste

Jennifer Readman

University of Central Lancashire, Preston, United Kingdom; jreadman@uclan.ac.uk

External Resource: Presentation



MS-79(69b)-680-005_b.pdf

12:05pm - 12:25pm

Crystal and Magnetic structures and Dielectric phase transition of the novel Organic-Inorganic Hybrid Halometallate compound: (quinuclidine)[FeCl₄]

Palmerina González-Izquierdo^{1,2}, Oscar Fabelo¹, Imanol de Pedro del Valle², María Teresa Fernández-Díaz¹, Laura Canadillas-Delgado¹, Garikoitz Beobide³, Manuel Sánchez Andújar⁴

¹ILL, Grenoble, France; ²CITIMAC, Universidad de Cantabria, Spain; ³Inorganic Chemistry, Universidad del País Vasco, EHU/UPV, Spain; ⁴Department of Chemistry, Universidade da Coruna, Spain; gonzalez-izquierdo@ill.fr

External Resource: Presentation



MS-79(69b)-155-006_b.pdf

MS-80: 4th generation SR and XFEL Facilities

Location: **Terrace 2A**

Session Chair: **Makina Yabashi**

Session Chair: **Sofia Diaz-Moreno**

Invited: **Jean Susini (France)**

Introduction

10:20am - 10:25am

Introduction to session

Makina Yabashi, Sofia Diaz-Moreno

10:20am - 12:45pm



MS-80-1811-001.pdf

10:25am - 10:55am

The ultra-low emittance synchrotron storage rings: a new paradigm for matter characterization.

Jean Susini

Synchrotron SOLEIL, Gif sur Yvette, France; jean.susini@synchrotron-soleil.fr

External Resource:



MS-80-1560-002_b.pdf

10:55am - 11:15am

Ultrafast structural changes in matter induced by intense X-ray free-electron laser pulses

Ichiro Inoue¹, Yuichi Inubushi^{1,2}, Taito Osaka¹, Toru Hara¹, Eiji Nishibori³, Makina Yabashi¹

¹RIKEN SPring-8 Center, 1-1-1 Kouto, Sayo, Hyogo 679-5148, Japan.; ²Japan Synchrotron Radiation Research Institute, Kouto 1-1-1, Sayo, Hyogo 679-5198, Japan; ³University of Tsukuba, Tsukuba, Ibaraki 305-8571, Japan.; inoue@spring8.or.jp

External Resource:



MS-80-1243-003_b.pdf

11:15am - 11:35am

Pink-beam serial femtosecond crystallography for accurate structure factor determination at an X-ray free electron laser

Karol Nass¹, Camila Bacellar¹, Claudio Cirelli¹, Florian Dworkowski¹, Yaroslav Gevorkov², Daniel James¹, Philip J. M. Johnson¹, Demet Kekilli¹, Gregor Knopp¹, Isabelle Martiel¹, Dmitry Ozerov¹, Alexandra Tolstikova², Laura Vera¹, Tobias Weinert¹, Oleksandr Yefanov², Joerg Standfuss¹, Sven Reiche¹, Christopher J. Milne¹

¹Paul Scherrer Institut, Forschungstrasse 111, Villigen, 5232, Switzerland; ²Center for Free-Electron Laser Science, Notkestrasse 85, Hamburg, 22607, Germany; karol.nass@psi.ch

External Resource:



MS-80-1191-004_b.pdf

11:35am - 11:55am

Towards a structural biology at organism relevant temperature and chemical conditions

John Richard Helliwell

University of Manchester, Manchester, United Kingdom; john.helliwell@manchester.ac.uk

External Resource:



MS-80-159-005_b.pdf

11:55am - 12:15pm

Ultrafast dynamical diffraction wavefronts in strained Si imagined with Tele-ptychography

Angel Rodriguez-Fernandez¹, Ana Diaz², Anand H. S. Iyer³, Mariana Verezhak², Klaus Wakonig², Magnus H. Colliander³, Dina Carbone⁴

¹Eu XFEL GmbH, Schenefeld, Germany; ²Paul Scherrer Institute, Villigen PSI, Switzerland; ³Chalmers University of Technology, Gothenburg, Sweden; ⁴MAX IV, Lund University, Lund, Sweden; angel.rodriguez-fernandez@xfel.eu

External Resource:



MS-80-772-006_b.pdf

Advances with EIGER2 (CdTe) detectors for Synchrotron and Laboratory

Stefan Brandstetter, Max Burian

Dectris Ltd, Baden-Daettwil, Switzerland; stefan.brandstetter@dectris.com

External Resource:



MS-80-874-007_b.pdf

12:45pm - 2:45pm

Lunch 6: Posters, lunches

Location: Exhibition and poster area



1:00pm - 2:30pm	ECA - SIG-11: ECA - SIG-11 Crystallography under Extreme Conditions Location: Club A Link	+
1:00pm - 2:30pm	ECA - SIG-13: ECA - SIG-13 Molecular Structure and Chemical Properties Location: virtual Link	+
1:00pm - 2:30pm	ECA - SIG-14: ECA - SIG-14 Dynamics, Disorder, Diffuse Scattering Location: Club D Link	+
1:00pm - 2:30pm	ECA - SIG-2: ECA - SIG-2 Quantum Crystallography Location: Club H Link	+
1:00pm - 2:30pm	ECA - SIG-9: ECA - SIG-9 Crystallographic Computing Location: virtual Link	+
1:00pm - 2:30pm	ECA-1: ECA EC meeting 2 Location: Club C Session Chair: Udo Heinemann Session Chair: Arie van der Lee ECA EC meeting	+
1:45pm - 2:45pm	ECA - SIG-7: ECA - SIG-7 Molecular Interaction and Recognition Location: virtual Link	+
2:45pm - 3:50pm	SMS-6: Spectroscopy applied to electrochemistry: operando studies Location: Club C Session Chair: Jasper Rikkert Plaisier Session Chair: Dibyendu Bhattacharyya Invited: Moniek Tromp (The Netherlands), Mahalingam Balasubramanian (USA) Introduction 2:45pm - 2:50pm Introduction to session <u>Jasper Rikkert Plaisier, Dibyendu Bhattacharyya</u>	+ +
	 SMS-6-1839-001.pdf	
	2:50pm - 3:20pm Operando X-ray Absorption Spectroscopy probing Dynamic Processes in Batteries Moniek Tromp University of Groningen, Groningen, Netherlands, The; moniek.tromp@rug.nl External Resource:  Presentation  SMS-6-1411-002_b.pdf	+ +
	3:20pm - 3:50pm Operando diagnostics of cathode materials based on novel sodium iron titanites Victor Vasilevich Shapovalov¹, Alexander Alexandrovich Guda¹, Vera Valerevna Butova¹, Abdelaziz Mohamed Aboraia¹, Igor Leonidovich Shukaev², Alexander Vladimirovich Soldatov¹ ¹ Smart Materials Research Institute, Southern Federal University, Rostov-on-Don, Russian Federation; ² Department of Chemistry, Southern Federal University, Rostov-on-Don, Russian Federation; viks@sfsu.ru  SMS-6-559-003_b.pdf	+ +
2:45pm - 5:10pm	MS-81: Nucleic acids and binding proteins structure and function Location: Club A Session Chair: Stephen Neidle Session Chair: Charles Bond Invited: Millie Georgiadis (USA), Liliya Yatsunyk (USA) 2:45pm - 2:50pm Introduction to session <u>Stephen Neidle, Charles Bond</u>	+ +
	 MS-81-1812-001.pdf	
	2:50pm - 3:20pm Non-canonical DNA structures and their interactions with small molecule ligands Liliya A. Yatsunyk, Dana Beseiso, Sawyer McCarthy, Erin Chen, Elizabeth Gallagher, Joanne Miao Swarthmore College, 500 College Ave, Swarthmore, PA, United States of America External Resource:  Presentation	+ +



MS-81-169-002_b.pdf

3:20pm - 3:50pm

Structural properties of Alien DNA, an alternative genetic system

Millie M. Georgiadis¹, Shuichi Hoshika², Steven Benner²

¹Indiana University School of Medicine, Indianapolis, Indiana, United States of America; ²Foundation for Applied Molecular Evolution, Alachua, Florida, United States of America

External Resource:



MS-81-1564-003_b.pdf

3:50pm - 4:10pm

APE1 Exonuclease Distinguishes Various DNA Substrates by an Induced Space-Filling Mechanism.

Tung-Chang Liu², Chun-Ting Lin¹, Kai-Cheng Chang¹, Kai-Wei Guo², Shuying Wang³, Jhih-Wei Chu⁴, Yu-Yuan Hsiao²

¹Department of Biological Science and Technology, National Yang Ming Chiao Tung University, Hsinchu 30068, Taiwan; ²Institute of Molecular Medicine and Bioengineering, National Chiao Tung University, Hsinchu 30068, Taiwan; ³Department of Microbiology and Immunology, College of Medicine, National Cheng Kung University, Tainan, Taiwan; ⁴Institute of Bioinformatics and Systems Biology, National Chiao Tung University, Hsinchu, 30068, Taiwan

External Resource:



MS-81-849-004_b.pdf

4:10pm - 4:30pm

Structural characterization of clinically reported missense mutations identified in BRCA1

Neha Mishra, Suchita Dubey, Ashok K Varma

Tata Memorial Centre Advanced Centre for Treatment, Research and Education in Cancer, Mumbai, India; neha.mish02@gmail.com

External Resource:



MS-81-738-005_b.pdf

4:30pm - 4:50pm

Solid-solid phase transition in adenine riboswitch crystals driven by large conformational changes induced by ligand

Jason R. Stagno¹, Saminathan Ramakrishnan¹, William F. Heinz², Valentin Magidson², Xiaobing Zuo³, Yun-Xing Wang¹

¹Center for Structural Biology, Centre for Cancer Research, National Cancer Institute, Frederick, MD-21702, USA.; ²Optical Microscopy and Analysis Laboratory, Cancer Research Technology Program, Frederick National Laboratory for Cancer Research, Frederick, MD 21702, USA.; ³X-ray Science Division, Argonne National Laboratory, Lemont, IL 60439, USA

External Resource:



MS-81-1306-006_b.pdf

Molecular mechanism of self-antigen recognition by the ligand binding domain of B cell inhibitory co-receptor CD72

Nobutaka Numoto¹, Kunio Hirata², Chizuru Akatsu³, Takeshi Tsubata³, Nobutoshi Ito¹

¹Department of Structural Biology, Medical Research Institute, Tokyo Medical and Dental University, Tokyo, Japan; ²RIKEN SPring-8 Center, Hyogo, Japan; ³Department of Immunology, Medical Research Institute, Tokyo Medical and Dental University, Tokyo, Japan

External Resource:



MS-81-1500-007_b.pdf

MS-82: Handling of big data in crystallography

Location: 223-4

Session Chair: **Wladek Minor**

Session Chair: **Brinda Vallat**

Introduction

2:45pm - 2:50pm

Introduction to session

Wladek Minor, Brinda Vallat



MS-82-1813-001.pdf

2:45pm - 5:10pm

2:50pm - 3:20pm

IRRC (https://proteindiffraction.org): Impact on quality of structures in PDB

Marek Grabowski, Marcin Cymborowski, David Cooper, Wladek Minor
UNIVERSITY OF VIRGINIA, Charlottesville, United States of America; marek@iwonka.med.virginia.edu

External Resource:



MS-82-1386-002_b.pdf

3:20pm - 3:50pm

A Gold Standard for the archiving of macromolecular diffraction data

Herbert J. Bernstein¹, Andreas Förster², Aaron S. Brewster³, Graeme Winter⁴

¹Ronin Institute for Independent Scholarship, c/o NSLS II, Brookhaven National Laboratory, Upton, NY, USA; ²DECTRIS Ltd., Täferweg 1, 5405 Baden-Dättwil, CH; ³Lawrence Berkeley National Laboratory, 1 Cyclotron Road, Berkeley, CA 94720, USA; ⁴Diamond Light Source Ltd, Harwell Science and Innovation Campus, Didcot OX11 0DE, UK; hbernstein@bnl.gov

External Resource:



MS-82-660-003_b.pdf



MS-82-660-003_c.pdf

3:50pm - 4:15pm

Data evaluation on the fly: Auto-Rickshaw at the MX beamlines of the Australian Synchrotron

Santosh Panjikar

Australian Synchrotron, ANSTO, Clayton, Australia; santoshp@ansto.gov.au

External Resource:



MS-82-1315-004_b.pdf

4:15pm - 4:40pm

Rapid response to biomedical challenges and threats

Wladek Minor¹, Mariusz Jaskolski², Alexander Wlodawer³, Zbigniew Dauter³, Joanna Macnar⁴, Dariusz Brzezinski⁵, David Cooper¹, Marcin Kowiel⁷, Mirosław Gilski², Ivan Shabalin¹, Marek Grabowski¹, Bernhard Rupp⁶

¹University of Virginia, Charlottesville, United States of America; ²A. Mickiewicz University, Poznan, Poland; ³National Cancer Institute, United States of America; ⁴University of Warsaw, Warsaw, Poland; ⁵Poznan University of Technology, Poznan, Poland; ⁶k.-k Hofkristallamt, United States of America; ⁷Polish Academy of Sciences, Poland; wladek@iwonka.med.virginia.edu

External Resource:



MS-82-1582-005_b.pdf

4:40pm - 5:05pm

Development of an on-the-fly data processing with information-lossless compression for CITIUS detectors at SPring-8

Toshiyuki Nishiyama Hiraki¹, Toshinori Abe^{1,2}, Mitsuhiro Yamaga^{1,2}, Takashi Sugimoto^{1,2}, Kyosuke Ozaki¹, Yoshiaki Honjo¹, Yasumasa Joti^{1,2}, Takaki Hatsui¹

¹RIKEN SPring-8 Center, Hyogo, Japan; ²Japan Synchrotron Radiation Research Institute, Hyogo, Japan; toshiyuki.nishiyama@riken.jp

External Resource:



MS-82-1044-006_b.pdf

MS-83: High pressure crystallography

Location: **Terrace 2A**

Session Chair: **Lars Ehm**

Session Chair: **Jon Henry Eggert**

Session Chair: **Vitali Prakapenka**

Session Chair: **Przemysław Dera**

Merged sessions

Invited: **June Wicks (USA)**, **Rachel Husband (Germany)**

Introduction

2:45pm - 2:50pm

Introduction to session

Lars Ehm, **Jon Henry Eggert**, **Vitali Prakapenka**, **Przemysław Dera**



MS-83-1814-001.pdf

2:45pm - 5:10pm

2:50pm - 3:20pm

Experimental measures of the orientation dependence of the B1-B2 transformation in shock-compressed MgO

June Ki Wicks

Johns Hopkins University, Baltimore, United States of America; wicks@jhu.edu

External Resource:



MS-83-1683-002_b.pdf

3:20pm - 3:50pm

Simultaneous imaging and diffraction of phase transitions at intermediate compression rates

Rachel J. Husband¹, Zsolt Jenei², Johannes Hagemann¹, Earl F. O'Bannon², William J. Evans², Andreas Schropp¹, Konstantin Glazyrin¹, Hanns-Peter Liermann¹

¹DESY, Notkestrasse 85, 2260 Hamburg, Germany; ²Lawrence Livermore National Laboratory, 7000 East Avenue, L-041 Livermore, CA 94550, USA; rachel.husband@desy.de

External Resource:



MS-83-1370-003_b.pdf

3:50pm - 4:10pm

Phase Changes in Dynamically Compressed Water

Michael G Stevenson¹, Lisa M V Zinta¹, Benjamin Heuser¹, Zhiyu He¹, Divyanshu Rajan¹, Mandy Bethkenhagen¹, Martin French¹, Armin Bergermann¹, Ronald Redmer¹, Thomas Cowan², Oliver Humphries², Julian Lütgert², Katja Voigt², Anja Schuster², Tommaso Vinci³, Emma E McBride⁴, Nicholas J Hartley⁴, Arianna Gleason-Holbrook⁴, Siegfried Glenzer⁴, Silvia Pandolfi⁴, Adrien Descamps⁴, Benjamin Ofori-Okai⁴, Christopher Schoenwaelder⁴, Griffin Glenn⁴, Luke B Fletcher⁴, Bob Nagler⁴, Hae Ja Lee⁴, Eric Galtier⁴, Dimitri Khaghani⁴, Jean-Alexis Hernandez⁵, Alessandra Ravasio³, Dominik Kraus^{1,2}

¹University of Rostock, Rostock, Germany; ²Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany; ³Laboratoire LULI, Ecole Polytechnique, Palaiseau, France; ⁴SLAC National Accelerator Laboratory, Menlo Park, USA; ⁵University of Oslo, Oslo, Norway; michael.stevenson@uni-rostock.de

External Resource:



MS-83-1119-004_b.pdf

4:10pm - 4:30pm

Investigations of the high-pressure, high-temperature behaviour of Au using laser-driven dynamic compression

Amy Coleman, Raymond Smith, Tom Lockard, Damian Swift, James McNaney

Lawrence Livermore National Laboratory, Livermore, United States of America; coleman55@llnl.gov

External Resource:



MS-83-990-005_b.pdf

4:30pm - 4:50pm

Mineral inclusions as models to characterize deviatoric stress in single crystals

Marta Morana¹, Ross J. Angel², Alice Girani¹, Mara Murri¹, Federico Alabarse³, Matteo Alvaro¹

¹University of Pavia, Pavia, Italy; ²Istituto di Geoscienze e Georisorse, Padua, Italy; ³Elettra Sincrotrone, Basovizza, Trieste, Italy; marta.morana01@universitadipavia.it

External Resource:



MS-83-395-006_b.pdf

4:50pm - 5:10pm

High-pressure low-temperature phase transitions and structural development in quasi-two-dimensional transition metal oxychlorides

Achim Mathias Schaller¹, Maxim Bykov^{2,3}, Elena Bykova², Konstantin Glazyrin⁴, Sander van Smaalen¹

¹University of Bayreuth, Laboratory of Crystallography, Bayreuth, Germany; ²Carnegie Institution of Washington, Geophysical Laboratory, Washington DC, USA; ³Howard University, Washington DC, USA; ⁴Photon Sciences, Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany; achim.schaller@uni-bayreuth.de

External Resource:



MS-83-187-007_b.pdf

MS-85: Science meets art: Crystallography and cultural heritage



Location: **Club H**

Session Chair: **Alicja Rafalska-Lasocha**

Session Chair: **Petr Bezdička**

Invited: **Koen Janssens (Belgium), Sebastian Bette (Germany)**

Introduction

2:45pm - 2:50pm

Introduction to session

Alicja Rafalska-Lasocha, Petr Bezdička



MS-85-1815-001.pdf

2:50pm - 3:20pm

Fingerprinting Natural Ultramarine in 15th-17th century Netherlandish paintings

Koen Henri JANSSENS^{1,4}, Steven De Meyer¹, Stijn Legrand¹, Frederik Vanmeert^{1,2}, Veronique Buecken³, Annelies van Loon⁴, Katrien Keune⁴

¹University of Antwerp, Antwerp, Belgium; ²Royal Institute for Cultural Heritage, Brussels, Belgium; ³Fine Arts Museum, Brussels, Belgium; ⁴Rijksmuseum, Amsterdam, The Netherlands; koen.janssens@uantwerpen.be

External Resource:



MS-85-1423-002_b.pdf

3:20pm - 3:50pm

The variety of calcium bearing efflorescence phases - An explanation by crystal chemistry

Sebastian Bette^{1,2}, Gerhard Eggert², Robert E. Dinnebier¹

¹Max-Planck-Institute for Solid State Research, Stuttgart, Germany; ²State Academy of Art and Design, Stuttgart, Germany; S.Bette@fkf.mpg.de

External Resource:



MS-85-579-003_b.pdf

3:50pm - 4:10pm

Why is heptagonal symmetry so rare in art and architecture?

Arie van der Lee

Institut Européen des Membranes, Université de Montpellier, ENSCM, CNRS, Montpellier, France; arie.van-der-lee@umontpellier.fr

External Resource:



MS-85-1183-004_b.pdf

4:10pm - 4:30pm

Crystallography vs. human masterpiece: $\text{Li}_{20}\text{Mg}_6\text{Cu}_{13}\text{Al}_{42}$, $\text{Mg}_9\text{Ni}_6\text{Ga}_{14}$ and $\text{Mg}_3\text{Ni}_2\text{Ga}$ structures vs. ivory puzzle balls

Grygoriy Dmytriv¹, Nazar Pavlyuk¹, Volodymyr Pavlyuk^{1,2}, Helmut Ehrenberg³

¹Ivan Franko National University of Lviv, Lviv, Ukraine; ²Częstochowa Jan Długosz University, Częstochowa, Poland; ³Karlsruhe Institute of Technology, Karlsruhe, Germany; gr_dmytriv@yahoo.com

External Resource:



MS-85-386-005_b.pdf

4:30pm - 4:50pm

Information theory based symmetry classifications of more or less 2D periodic patterns in Islamic building ornaments and Hans Hinterreiter's graphic art

Peter Moeck

Portland State University, PORTLAND, Oregon, USA; pmoeck@pdx.edu

External Resource:



MS-85-116-006_b.pdf

4:50pm - 5:10pm

Laboratory X-ray powder diffraction as a useful tool for identification of pigments and degradation products in portrait miniatures painted on ivory

Eva Kočí¹, Petr Bezdička¹, Silvia Garrappa¹, David Hradil¹, Janka Hradilová², Michal Pech²

¹Institute of Inorganic chemistry of the Czech Academy of Sciences, ALMA Laboratory, Husinec-Řež 1001, 250 68 Husinec-Řež, Czech Republic; ²Academy of Fine Arts in Prague, ALMA Laboratory, Veletřní 65, 170 00 Praha 7, Czech Republic; eva.koci@iic.cas.cz

External Resource:



MS-85-1053-007_b.pdf

MS-86: Modular structure of inorganic and mineral compounds



Location: **Club D**

Session Chair: **Isabella Pignatelli**

Session Chair: **Berthold Stöger**

Invited: **Olivier Perez (France)**, **Marie Colmont (France)**

Introduction

2:45pm - 2:50pm

Introduction to session

Isabella Pignatelli, Berthold Stöger



MS-86-1816-001.pdf

2:50pm - 3:20pm

Designing Composite Spin Chain Structures Built up of Dimeric and Trimeric Polyhedral Units: The oxides $A_{1+y}[(Mn_{1-x}Co_x)_{1-z}Z]O_3$ (A=Ca, Sr; x = 3/8).



Olivier Perez¹, Vincent Caignaert¹, Bernard Raveau¹, Vincent Hardy Hardy¹, Nahed Sakly¹, MD Motin Seikh²
¹CRISMAT, CNRS-ENSICAEN, 6 Bd du Maréchal Juin, 14050 Caen Cedex, France; ²Department of Chemistry, Visva-Bharati University, Santiniketan 731235, West Bengal, India; olivier.perez@ensicaen.fr

External Resource:



MS-86-1626-002_b.pdf

3:20pm - 3:50pm

Diffraction enhancement of symmetry and modular structures



Akihiro Umayahara^{1,2}, Bernd Souvignier¹, Massimo Nespolo²

¹Radboud University, Faculty of Science, Mathematics and Computing Science, Institute for Mathematics, Astrophysics and Particle Physics, Postbus 9010, 6500 GL Nijmegen, The Netherlands.; ²Université de Lorraine, Vandoeuvre lès Nancy, France; akihiro.umayahara@univ-lorraine.fr

External Resource:



MS-86-863-003_b.pdf

3:50pm - 4:15pm

Polytypism in cronstedtite; how various stacking sequences of layers affect diffraction pattern



Jiří Hybler

Institute of Physics of the Czech Academy of Sciences, Prague 8, Czech Republic; hybler@fzu.cz

External Resource:



MS-86-653-004_b.pdf

4:15pm - 4:40pm

Binary beryllium pnictides: ordered and disordered coloring variants of the diamond structure



Alexander Feige, Marvin Michak, Maxim Grauer, Daniel Günther, Lennart Staab, Christopher Benndorf, Oliver Oeckler
Leipzig University, Faculty of Chemistry and Mineralogy, Leipzig, Germany; alexander.feige@t-online.de

External Resource:



MS-86-773-005_b.pdf



MS-86-773-005_c.pptx

MS-87: Topological materials



Location: **Terrace 2B**

Session Chair: **Yugui Yao**

Session Chair: **Wenhui Duan**

Session Chair: **Avadh B. Saxena**

Invited: **Tomasz Dietl (Poland)**, **Xiang Li (China)**

2:45pm - 2:50pm

Introduction to session

Catherine Pappas, Yugui Yao, Wenhui Duan, Avadh B Saxena



2:45pm - 5:10pm

2:45pm - 5:10pm



MS-87-1817-001.pdf

2:50pm - 3:20pm

Phase separations and nematicity of transition metal impurities

Tomasz Dietl^{1,2}

¹International Research Centre MagTop, Institute of Physics, Polish Academy of Sciences, Warsaw, Poland; ²WPI-Advanced Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan; dietl@MagTop.ifpan.edu.pl

External Resource:



MS-87-641-002_b.pdf

3:20pm - 3:50pm

Pressure-induced phase transitions and superconductivity in a black phosphorus single crystal

Xiang Li

Beijing Institute of Technology, Beijing, China, People's Republic of; xiangli@bit.edu.cn

External Resource:



MS-87-604-003_b.pdf

3:50pm - 4:10pm

Unconventional states and topological defects in Fe-langasite

Maxim V. Mostovoy, Evgenii O. Barts

Zernike Institute for Advanced Materials, University of Groningen, The Netherlands; e.barts@rug.nl

External Resource:



MS-87-1122-004_b.pdf

4:10pm - 4:30pm

Magnetic excitations and structure of the topological semimetal YbMnSb₂

Siobhan Maeve Tobin¹, Jian-Rui Soh², Hao Su³, Bachir Ouladdiaf⁴, Andrea Piovano⁴, Yang-Feng Guo³, Dharmalingam Prabhakaran¹, Andrew Timothy Boothroyd¹

¹University of Oxford, Oxford, United Kingdom; ²Institute of Physics, École Polytechnique Fédéral de Lausanne, Switzerland; ³School of Physical Science and Technology, ShanghaiTech University, China; ⁴Institut Laue Langevin (ILL), France; siobhan.tobin@physics.ox.ac.uk

External Resource:



MS-87-693-005_b.pdf

4:30pm - 4:50pm

Occupancy disorder and magnetism in tetradymite based topological insulators

Laura Christina Folkers^{1,2,3}, Anna Isaeva^{3,4}

¹Technical University Dresden, Dresden, Germany; ²Institute for Solid State and Materials Physics, TU Dresden, Germany; ³Leibniz Institute for Solid State and Materials Research, Dresden, Germany; ⁴University of Amsterdam, Amsterdam, The Netherlands; laura_christina.folkers1@tu-dresden.de

External Resource:



MS-87-1849-006_b.pdf

4:50pm - 5:10pm

Topological analysis of local heteropolyhedral substitutions in the eudialyte-related structures

Sergey Aksenov^{1,2}, Natalia Kabanova^{1,3}, Nikita Chukanov^{4,5}, Vladislav Blatov³, Sergey Krivovichev^{6,7}

¹Laboratory of Nature-Inspired Technologies and Environmental Safety of the Arctic, Kola Science Centre, Russian Academy of Sciences, Apatity, Russian Federation; ²Geological Institute, Kola Science Centre, Russian Academy of Sciences, Apatity, Russian Federation; ³Samara Center for Theoretical Materials Science, Samara State Technical University, Samara, Russian Federation; ⁴Institute of Problems of Chemical Physics, Russian Academy of Sciences, Chernogolovka, Russian Federation; ⁵Faculty of Geology, Moscow State University, Vorobievsky Gory, Moscow, Russian Federation; ⁶Nanomaterials Research Centre, Kola Science Center, Russian Academy of Sciences, Apatity, Russian Federation; ⁷Department of Crystallography, Institute of Earth Sciences, St Petersburg State University, St Petersburg, Russian Federation; aks.crys@gmail.com

External Resource:





MS-87-1847-007_b.pdf

MS-88: Quantum crystallography research

Location: **Club B**

Session Chair: **Yu-Sheng Chen**

Session Chair: **Katarzyna N. Jarzemska**

Invited: **Sophie E. Canton** (Hungary), **Simon Grabowsky** (Switzerland)

2:45pm - 5:10pm

Introduction

2:45pm - 2:50pm

Introduction to session

Yu-Sheng Chen, **Katarzyna N. Jarzemska**



MS-88-1818-001.pdf

2:50pm - 3:20pm

Synchrotron experiments revealing the similarities and differences between crystal and enzyme environmental effects on the electron densities of protease inhibitors and ibuprofen derivatives

Simon Grabowsky

University of Bern, Bern, Switzerland; simon.grabowsky@dcb.unibe.ch

External Resource:



MS-88-790-002_b.pdf

3:20pm - 3:50pm

Visualizing the multiscale structural dynamics of photoexcited molecular complexes with ultrafast hard X-rays

Sophie Canton

European XFEL, Schenefeld, Germany; sophie.canton@xfel.eu

External Resource:



MS-88-1565-003_b.pdf

3:50pm - 4:10pm

Ultrafast photocrystallographic and spectroscopic studies of selected coinage-metal coordination compounds

Piotr Łaski¹, **Jakub Drapała**², **Radosław Kamiński**¹, **Krzysztof Durka**², **Katarzyna Natalia Jarzemska**¹

¹University of Warsaw, Warsaw, Poland; ²Warsaw Institute of Technology, Poland; piotr.laski@gmail.com

External Resource:



MS-88-549-004_b.pdf

4:10pm - 4:30pm

Electronic structure of (MePh₃P)₂[Ni^{II}(bdtCl₂)₂] · (CH₃)₂SO and (MePh₃P)[Ni^{III}(bdtCl₂)₂], (bdtCl₂ - 3,6-dichlorobenzene-1,2-dithiolate)

Jozef Kozisek

STU Bratislava, Bratislava, Slovak Republic; jozef.kozisek@stuba.sk

External Resource:



MS-88-1248-005_b.pdf

4:30pm - 4:50pm

Unusual carbonyl interactions in co-crystals of urea and dicarboxylic acids

Anna Malgorzata Krawczuk¹, **Mariusz Mitoraj**²

¹University of Göttingen, Göttingen, Germany; ²Jagiellonian University in Krakow, Krakow, Poland; anna.krawczuk@uni-goettingen.de

External Resource:



MS-88-935-006_b.pdf

4:50pm - 5:10pm

Testing various variants of Hirshfeld atom like refinement.

Michał Chodkiewicz, Magdalena Woińska, Sylwia Pawłędzio, Leonid Patrikeev, Krzysztof Woźniak
University of Warsaw, Warszawa, Poland; ml.chodkiewicz@uw.edu.pl

External Resource:  Presentation



MS-88-960-007_b.pdf

SF-6: Software Fayre 6

Location: 221-2

Session Chair: **Martin Lutz**

Session Chair: **Claudia Millán**

<http://www.cryst.chem.uu.nl/lutz/>

2:55pm - 3:40pm

AUSPEX: Finding pathologies in macromolecular X-ray data

Yunyun Gao

University Hamburg, Hamburg, Germany; yunyun.gao@cfel.de

External Resource:  Presentation

3:40pm - 4:25pm

winPSSP: solving organic materials from powder diffraction

SILVINA PAGOLA

Old Dominion University, Williamsburg, United States of America; spagola@odu.edu

External Resource:  Presentation

4:25pm - 5:10pm

Eval15: Intensity integration of area detector images

Martin Lutz

Utrecht University, Utrecht, Netherlands, The; m.lutz@uu.nl

External Resource:  Presentation

5:10pm - 5:55pm

Yell: Diffuse scattering analysis in single crystals

Arkadiy Simonov

ETH Zurich, Zurich, Switzerland; arkadiy.simonov@mat.ethz.ch

External Resource:  Presentation

SMS-5: Advances in data and model validation in biomolecular Small-Angle Scattering: Impacts on data and meta-data recording and data archiving

Location: **Club C**

Session Chair: **Javier Perez**

Session Chair: **Thomas Weiss**

Invited: **Dina Schneidman (Israel)**, **Thomas Grant (USA)**

Introduction

3:55pm - 4:00pm

Introduction to session

Javier Perez



SMS-5-1840-001.pdf

4:00pm - 4:30pm

Representing low-resolution electron density maps from solution scattering data

Thomas Grant

University at Buffalo, Buffalo, United States of America; tdgrant@buffalo.edu

External Resource:  Presentation



SMS-5-1136-002_b.pdf

4:30pm - 5:00pm

Integrative modeling of structure and dynamics of macromolecules based on SAXS profiles and cross-linking mass spectrometry

Dina Schneidman

The Hebrew University of Jerusalem, Jerusalem, Israel; dina.schneidman@mail.huji.ac.il

2:55pm - 5:55pm

3:55pm - 5:25pm



SMS-5-1049-003_b.pdf

5:10pm - 6:10pm

Afternoon break 6: Poster session C2, coffee/tea

Location: **Exhibition and poster area**



Poster - 41 Receptors: Structural biology of receptors, membrane proteins



Session Chair: **SUSAN KAY BUCHANAN**

Session Chair: **Michael Parker**

5:10pm - 6:10pm

Poster session abstracts

Radomír Kužel



Poster - 41 Receptors-1968-001.pdf

Structural anomalies in the Eph receptor due to clinically relevant mutations and the subsequent effect on kinase domain

Shubhashish Chakraborty^{1,2}, Ashok Kumar Varma^{1,2}

¹Advanced centre for Treatment, Research and Education in cancer, Kharghar, Navi Mumbai, Maharashtra – 410210, INDIA; ²Homi Bhabha National Institute, Training School Complex, Anushaktinagar, Mumbai, Maharashtra – 400094, INDIA;

schakraborty@actrec.gov.in

External Resource:



Poster - 41 Receptors-709-002_b.pdf

Influence of glycosylation on the structure of human natural killer cell receptor NKp30 in complex with its tumor ligand B7-H6

Tereza Skalova¹, Ondřej Škořepa², Barbora Kalousková², Jan Bláha², Celeste Abreu², Jan Dohnálek¹, Ondřej Vaněk²

¹Institute of Biotechnology CAS, v.v.i., Vestec, Czech Republic; ²Department of Biochemistry, Faculty of Science, Charles University Prague, Hlavova 8, 128 40 Praha, Czech Republic

External Resource:



Poster - 41 Receptors-998-003_b.pdf

CD4⁺ T cell recognition of pneumolysin, a pore-forming cytotoxin derived from *Streptococcus pneumoniae* presented by a common HLA allotype

Lisa Ciacchi¹, Martijn D. B. van de Garde², Jan Petersen¹, Carine Farenc¹, Martien C. M. Poelen², Hugh H. Reid¹, Kristin Ladell³, David A. Price³, Cecile A. C. M. van Els², Jamie Rossjohn¹

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External Resource:



Poster - 41 Receptors-1467-004_b.pdf

Molecular characterization of the native (non-linked) CD160-HVEM protein complex revealed by initial crystallographic analysis

Simona Lenhartová¹, Marek Nemčovič², Radka Šebová¹, Mário Benko¹, Dirk Zajonc^{3,4}, Ivana Nemčovičová¹

¹Biomedical Research Center, Slovak Academy of Sciences, Bratislava, Slovak Republic; ²Institute of Chemistry, Slovak Academy of Sciences, Bratislava, Slovakia; ³Division of Immune Regulation, La Jolla Institute for Immunology, La Jolla, CA, USA; ⁴Cancer Immunology Discovery, Pfizer Inc., San Diego, CA, USA

External Resource:



Poster - 41 Receptors-1627-005_b.pdf

Structure-based drug discovery enabled for membrane protein targets

Michael Hennig

leadXpro AG, Villigen, Switzerland

External Resource:



Poster - 41 Receptors-1534-006_b.pdf

Optimization of the NZ-1 labeling technique for the application to 3D structure analysis

Rie Aruga¹, Risako Tamura-Sakaguchi¹, Mika Hirose², Toru Ekimoto¹, Rika Oi¹, Mika K. Kaneko³, Yukinari Kato^{3,4}, Mitsunori Ikeguchi^{1,5}, Kenji Iwasaki⁶, Terukazu Nogi¹

¹Graduated School of Medical Life Science, Yokohama-city University, Japan; ²Institute for Protein Research, Osaka University, Japan; ³Department of Antibody Drug Development, Tohoku University Graduate School of Medicine, Japan; ⁴New Industry Creation Hatchery Center, Tohoku University, Japan; ⁵Center for Computational Science, RIKEN, Japan; ⁶Life Science Center for Survival Dynamics, Tsukuba Advanced Research Alliance (TARA), University of Tsukuba, Japan

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Poster - 41 Receptors-1453-007_b.pdf

Structure, function and evolution of the orally active insecticidal toxin complex, YenTc

Sarah Piper^{1,2}, Lou Brillault^{1,2}, Joseph Box¹, Yu Shang Low¹, Irene Chassagnon¹, Gabriel Foley¹, Nadezhda Aleksandrova¹, Lauren Hartley-Tassell⁴, Cassandra Pegg¹, Ben Schulz¹, Thomas Ve⁴, Shaun Lott³, Mark Hurst⁵, Michael Landsberg^{1,2}

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Poster - 41 Receptors-1633-008_b.pdf

Understanding the structural basis of TIR-domain assembly formation in TRAM- and TRIF- dependent TLR signalling

Mengqi Pan, Andrew Hedger, Jeff Nanson, Bostjan Kobe

the University of Queensland, St Lucia, Australia; m.pan@uq.edu.au

External Resource:  Presentation



Poster - 41 Receptors-1729-009_b.pdf

Structural basis of higher-order assembly formation in Toll-like receptors 1,2 and 6 signaling pathway

YAN LI

The University of Queensland, St Lucia, Australia; yan.li9@uqconnect.edu.au



Poster - 41 Receptors-1920-010_b.pdf

Poster - 42 Enzymes: Structural biology of enzymes

Session Chair: **Mirjam Czjzek**



5:10pm - 6:10pm

Poster session abstracts

Radomír Kužel



Poster - 42 Enzymes-1969-001.pdf

Structural characterisation of mitochondrial complex IV assembly factors

Shadi Maghool¹, Luke Formosa², Dinesha Cooray³, David Stroud⁴, David Aragão⁵, Michael Ryan², Megan Maher¹

¹School of Chemistry and The Bio21 Molecular Science and Biotechnology Institute, The University of Melbourne, Parkville, Australia; ²Department of Biochemistry and Molecular Biology, Biomedicine Discovery Institute, Monash University, Clayton 3800, Australia; ³Department of Biochemistry and Genetics, La Trobe Institute for Molecular Science, La Trobe University, Melbourne 3086, Australia; ⁴Department of Biochemistry and Molecular Biology and The Bio21 Molecular Science and Biotechnology Institute, The University of Melbourne, Parkville, Victoria 3010, Australia; ⁵Diamond Light Source, Harwell Science and Innovation Campus, Didcot, UK; shadi.maghool@unimelb.edu.au

External Resource:  Presentation



Poster - 42 Enzymes-250-002_b.pdf

Chemical biology and structural studies on the mechanism of regulation of phosphoinositide-dependent protein kinase 1 (PDK1)

Lissy Z. F. Gross¹, Mariana Sacerdoti¹, Alejandro E. Leroux¹, Abhijeet Ghode⁴, Ganesh S. Anand⁴, Jörg O. Schulze², Melissa A. Graewert⁵, Dmitri I. Svergun⁵, Sebastian Klinke³, Ricardo M. Biondi^{1,2}

¹IBioBA - CONICET - Partner Institute of the Max Planck Society, Buenos Aires, Argentine Republic; ²Department of Internal Medicine I, Universitätsklinikum Frankfurt, Germany; ³Leloir Institute - CONICET, Buenos Aires, Argentine Republic; ⁴Department of Biological Sciences, National University of Singapore, Singapore; ⁵European Molecular Biology Laboratory (EMBL), DESY Hamburg, Germany; lgross@ibioba-mpsp-conicet.gov.ar

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Poster - 42 Enzymes-283-003_b.pdf

Structure of the *Caulobacter Crescentus* suppressor of copper sensitivity protein C

Guillaume A. Petit¹, Karrera Y. Djoko², Jennifer L. Martin^{1,3}, Maria A. Halli¹

¹Griffith Institute for Drug Discovery, Griffith University, Nathan, QLD, Australia; ²Department of Biosciences, Durham University, UK;

³Vice-Chancellor's Unit, University of Wollongong, NSW, Australia

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Poster - 42 Enzymes-890-004_b.pdf

The structural panorama of L-asparaginases includes an alien from nitrogen-fixing bacteria

Mariusz Jaskolski¹, Joanna Loch², Mirek Gilski¹, Barbara Imiolczyk³

¹Faculty of Chemistry, A.Mickiewicz University, Poznan, Poland, Institute of Bioorganic Chemistry, Polish Academy of Sciences,

Poznan, Poland; ²Faculty of Chemistry, Jagiellonian University, Cracow, Poland; ³Institute of Bioorganic Chemistry, Polish Academy of Sciences, Poznan, Poland

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Poster - 42 Enzymes-121-005_b.pdf

Structures of a DYW domain shed first light on a unique plant RNA editing regulation principle

Mizuki Takenaka¹, Sachi Takenaka¹, Tatjana Barthel², Brody Frink¹, Sascha Haag³, Daniil Verbitskiy³, Bastian Oldenkott⁴, Mareike Schallenberg-Rüdinger⁴, Christian Feiler², Manfred S. Weiss², Gottfried J. Palm⁵, **Gert Weber²**

¹Department of Botany, Graduate School of Science, Kyoto University, Kyoto, Japan; ²Helmholtz-Zentrum-Berlin (HZB), Berlin, Germany; ³Molekulare Botanik, Universität Ulm, Germany; ⁴IZMB – Institut für Zelluläre und Molekulare Botanik, Abt. Molekulare Evolution, University of Bonn, Bonn, Germany; ⁵University of Greifswald, Molecular Structural Biology, Greifswald, Germany

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Poster - 42 Enzymes-905-006_b.pdf

Seeing is believing: glycosylation in the crystal structure of human myeloperoxidase

Lucas Krawczyk¹, Shubham Semwal¹, Goedeke Roos¹, Pierre Van Antwerpen², **Julie Maria Jozefa Bouckaert¹**

¹Centre National de REcherche Scientifique, Villeneuve d'Ascq, France; ²Laboratory of Pharmaceutical Chemistry and Analytical Platform, Faculty of Pharmacy, Université libre de Bruxelles, CP205/05, Boulevard du Triomphe, 1050 Brussels, Belgium

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Poster - 42 Enzymes-987-007_b.pdf

14-3-3 protein dependent modulation of ubiquitin ligase Nedd4-2

Pavel Pohl^{1,2}, Tomáš Obšil^{1,3}, Veronika Obšilová¹

¹Institute of physiology, CAS, Vestec, Czech Republic; ²Second Faculty of Medicine, Charles University in Prague, Czech Republic;

³Dept. of Physical and Macromolecular Chemistry, Faculty of Science, Charles University in Prague, Czech Republic

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Poster - 42 Enzymes-982-008_b.pdf

Bacillithiol disulfide reductase Bdr - insight into a new type of FAD-containing NADPH-dependent oxidoreductases

Marta Hammerstad¹, Ingvald Gudim¹, **Hans-Petter Hersleth^{1,2}**

¹University of Oslo, Department of Biosciences, Oslo, Norway; ²University of Oslo, Department of Chemistry, Oslo, Norway

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Poster - 42 Enzymes-798-009_b.pdf

Exploring Polysaccharide lyases of PL-5 family through the lens of structure, function, and dynamics

Prerana Dash^{1,2}, Rudresh Acharya^{1,2}

¹National Institution of science education and research, Bhubaneswar, India; ²Homi Bhabha National Institute, Training School Complex, Anushakti Nagar, Mumbai 400094, Maharashtra, India

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Poster - 42 Enzymes-661-010_b.pdf

Structural and functional characterization of a DNA binding protein of pIP501– a broad-host-range plasmid

Tamara Margot Isamel Berger¹, Nina Gubensäk¹, Walter Keller¹, Verena Kohler²

¹University of Graz, Graz, Austria; ²University of Stockholm, Stockholm, Sweden

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Poster - 42 Enzymes-1267-011_b.pdf



Poster - 42 Enzymes-1267-011_c.pdf

First crystallographic study of a glutathione transferase from cyanobacteria

Eva Mocchetti¹, Arnaud Hecker², Benoît Guillot¹, Sandrine Mathiot¹, Franck Chauvat³, Corinne Cassier-Chauvat³, Claude Didierjean¹

¹CRM2, UL, CNRS, Nancy, France; ²IAM, UL, INRAE, Nancy, France; ³I2BC, UPS, CNRS, CEA, Paris-Saclay, France

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Poster - 42 Enzymes-1433-012_b.pdf

Structural insights into the ferroxidase and iron sequestration mechanisms of ferritin from *Caenorhabditis elegans*

Tess R. Malcolm¹, Sanjeedha Mohamed Mubarak¹, Eric Hanssen², Hamish G. Brown², Gawain McColl³, Megan J. Maher^{1,4}, Guy N.L. Jameson¹

¹Bio21 Molecular Science and Biotechnology Institute, Parkville, Australia; ²Ian Holmes Imaging Centre, Bio21 Molecular Science and Biotechnology Institute, University of Melbourne, Parkville, Victoria, Australia; ³The Florey Institute of Neuroscience and Mental Health, The University of Melbourne, Parkville, Victoria, Australia; ⁴Department of Biochemistry and Genetics, La Trobe Institute for Molecular Science, La Trobe University, Melbourne, Victoria, Australia

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Poster - 42 Enzymes-1344-013_b.pdf

Precise Redox-dependent Structural Change of the plant-type Ferredoxin revealed by X-ray structures at 0.77 Å resolution, originated and propagating from the [2Fe-2S] cluster

Yusuke Ohnishi^{1,2}, Hideki Tanaka¹, Genji Kurisu¹

¹Institute for Protein Research, Osaka University, 3-2 Yamadaoka, Suita city, Osaka 565-0871, Japan; ²School of Pharmaceutical Sciences, Wakayama Medical University, 25-1 Shichibancho, Wakayama city, Wakayama 640-8156, Japan

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Poster - 42 Enzymes-1446-014_b.pdf

Crystal structure of carbohydrate esterase SmAcE1 from *Sinorhizobium meliloti*

Changsuk Oh¹, Truc Kim¹, T. Doohun Kim², Kyeong Kyu Kim¹

¹Department of Precision Medicine, Sungkyunkwan University, Suwon, Korea, Republic of Korea; ²Department of Chemistry, College of Natural Science, Sookmyung Women's University, Seoul, 04310, Republic of Korea; csoh@skku.edu

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Poster - 42 Enzymes-1561-015_b.pdf

Half way to hypusine. Structural characterization of human deoxyhypusine synthase.

Elżbieta Wator, Piotr Wilk, Przemysław Grudnik

Malopolska Centre of Biotechnology, Jagiellonian University, Krakow, Poland

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Poster - 42 Enzymes-1609-016_b.pdf

On substrate binding cavity of hyoscyamine 6 β -hydroxylase from devil's trumpet

Anna Kluza¹, Beata Mrugała¹, Katarzyna Kurpiewska^{1,2}, Przemysław J Porebski^{1,3}, Ewa Niedziałkowska^{1,3}, Wlodek Minor³, Manfred S Weiss⁴, Maksymilian Chruszcz⁵, Tomasz Borowski¹

¹Jerzy Haber Institute of Catalysis and Surface Chemistry, Polish Academy of Sciences, Krakow, Poland; ²Department of Crystal Chemistry and Crystal Physics, Faculty of Chemistry, Jagiellonian University, Krakow, Poland; ³Department of Molecular Physiology and Biological Physics, University of Virginia, Charlottesville, VA, USA; ⁴Macromolecular Crystallography, Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany; ⁵Department of Chemistry and Biochemistry, University of South Carolina, Columbia, SC, USA

External Resource:  Presentation



Poster - 42 Enzymes-1541-017_b.pdf

Control of hydroxylation regioselectivity by hyoscyamine 6 β -hydroxylase as revealed by crystallographic and QM/MM studies

Zuzanna Wojdyła, Anna Kluza, Tomasz Borowski

Jerzy Haber Institute of Catalysis and Surface Chemistry Polish Academy of Sciences, Krakow, Poland; zuzanna.wojdyła@ikifp.edu.pl

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Poster - 42 Enzymes-1524-018_b.pdf

Domain movements of NADPH-cytochrome P450 oxidoreductase (CPR) are required for the smooth electron transfer from CPR to heme-heme oxygenase-1 (HO-1) complex

Masakazu Sugishima¹, Junichi Taira², Mikuru Iijima³, Hideaki Sato¹, Kei Wada⁴, Masato Noguchi¹, Keiichi Fukuyama⁵, Mitsunori Takano³, Hiroshi Sakamoto², Ken Yamamoto¹

¹Kurume University School of Medicine, Kurume, Japan; ²Kyushu Institute of Technology, Iizuka, Japan; ³Waseda University, Tokyo, Japan; ⁴University of Miyazaki, Miyazaki, Japan; ⁵Osaka University, Toyonaka, Japan

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Poster - 42 Enzymes-1487-019_b.pdf

Conservation of a glutamate residue in ATP-citrate lyase and succinyl-CoA synthetase

Marie Elizabeth Fraser, Ji Huang

University of Calgary, Calgary, Canada



Poster - 42 Enzymes-1622-020_b.pdf

Monitoring the crystallization of two enzymes in real time by dynamic light-scattering

Kévin Rollet^{1,2}, Raphaël de Wijn¹, Sylvain Engilberge³, Alastair G. McEwen⁴, Oliver Hennig², Heike Betet², Mario Möri², François Riobé⁵, Olivier Maury⁵, Philippe Bénas¹, Bernard Lorber¹, Claude Sauter¹

¹Université de Strasbourg, ARN, CNRS UPR9002, IBMC, Strasbourg, France; ²Institute for Biochemistry, Leipzig University, Leipzig, Germany; ³Université Grenoble Alpes, CEA, CNRS, IBS, Grenoble, France; ⁴Université de Strasbourg, IGBC, CNRS UMR 7104, INSERM U 1258, Illkirch, France; ⁵Université Lyon 1, ENS Lyon, CNRS-UMR 5182, Lyon, France

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Poster - 42 Enzymes-1472-021_b.pdf

Investigating The Structural Dynamics of the Water and Proton Channels Using snap-shots of Photosystem II

Mohamed Ibrahim

HU-Berlin, Berlin, Germany

External Resource:  Presentation



Poster - 42 Enzymes-1719-022_b.pdf

Poster - 43 Nucleic acid: Nucleic acids and binding proteins structure and function

Session Chair: **Charles Bond**

Session Chair: **Stephen Neidle**



5:10pm - 6:10pm

Introduction

Poster session abstracts

Radomír Kužel



Poster - 43 Nucleic acid-1970-001.pdf

Biophysical characterization of the interaction between Forkhead Box O4 (FOXO4) and p53 transcription factors

Raju Mandal¹, Klara Kohoutova^{1,2}, Olivia Petrvalska^{1,2}, Matej Horvath¹, Václav Veverka^{3,4}, Veronika Obsilova², Tomas Obsil^{1,2}

¹Department of Physical and Macromolecular Chemistry, Faculty of Science, Charles University, Prague, Czech Republic; ²Department of Structural Biology of Signaling Proteins, Division BIOCEV, Institute of Physiology of the Czech Academy of Sciences, 252 50 Vestec, Czech Republic; ³Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences, Prague, Czech Republic;

⁴Department of Cell Biology, Faculty of Science, Charles University, Prague, Czech Republic

External Resource: Presentation



Poster - 43 Nucleic acid-1505-002_b.pdf

Structural basis for the specific binding between metal ion and chemically modified mismatched base pairs

Kei Hirabayashi¹, Saki Adachi¹, Akira Ono², Jiro Kondo³, Hidetaka Torigoe¹

¹Department of Applied Chemistry, Faculty of Science, Tokyo University of Science, Tokyo 162-8601, Japan; ²Department of Material & Life Chemistry, Faculty of Engineering, Kanagawa University, Yokohama 221-8686, Japan; ³Department of Materials and Life Sciences, Faculty of Science and Technology, Sophia University, Tokyo 102-8554, Japan

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Poster - 43 Nucleic acid-1515-003_b.pdf

Structural and Functional Studies of TBEV Non-Structural Protein 5

Petra Havlíčková¹, Joel A. Crossley¹, Zdeno Gardian^{1,2}, Ivana Kutá Smatanová¹, Zdeněk Franta¹

¹Faculty of Science, University of South Bohemia in České Budějovice, České Budějovice, Czech Republic; ²Institute of Parasitology, Biology Center of the Czech Academy of Sciences, České Budějovice, Czech Republic

External Resource: Presentation



Poster - 43 Nucleic acid-1613-004_b.pdf

Lipopolysaccharide Recognition by human Surfactant Protein D.

William Anthony Neale¹, Jens Madsen², Howard Clark², Annette Shrive¹, Trevor Greenhough¹

¹Keele University, Staffordshire, United Kingdom; ²EGA Institute for Women's Health, University College London, United Kingdom

External Resource: Presentation



Poster - 43 Nucleic acid-1502-005_b.pdf

Poster - 44 Art: Crystallography in art and archaeology

Session Chair: **Petr Bezdička**

Session Chair: **David Hradil**



5:10pm - 6:10pm

Poster session abstracts

Radomír Kužel



Poster - 44 Art-1971-001.pdf

Characterization of metal carboxylates relevant for degradation of oil paintings by complementary XRPD and ssNMR

Ruslan Barannikov^{1,2}, Silvie Švarcová¹, Eva Kočí¹, Petr Bezdička¹, Libor Kobera³, Jan Rohlíček⁴, Jiří Plocek¹

¹Institute of Inorganic Chemistry of the Czech Academy of Sciences, ALMA Laboratory, Husinec-Řež 1001, 250 68 Husinec-Řež, Prague, Czech Republic; ²Department of Inorganic Chemistry, Faculty of Science, Charles University in Prague, Hlavova 2030/8, 128 43 Prague 2, Czech Republic; ³Institute of Macromolecular Chemistry of the Czech Academy of Sciences, Heyrovského nám. 2, 162 06 Praha 6, Czech Republic; ⁴Institute of Physics of the Czech Academy of Sciences, Na Slovance 1999/2, 182 21 Praha 8, Czech Republic; ruslan-kz94@mail.ru

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Poster - 44 Art-858-002_b.pdf

Meaning of Wenzel Jamnitzer's treatise *Perspectiva corporum regularium* (Nürnberg, 1568) and its relationship to history of modern science

Jan Fábry

Institute of Physics of the Czech Academy of Sciences, Praha 8, Czech Republic; fabry@fzu.cz

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Poster - 44 Art-607-003_b.pdf

Poster - 45 Minerals: Complex structures of minerals and inorganic materials



Session Chair: **Marie Colmont**

Session Chair: **Sergey V. Krivovichev**

Session Chair: **Milan Rieder**

5:10pm - 6:10pm

Poster session abstracts

Radomír Kužel



Poster - 45 Minerals-1972-001.pdf

The crystal structure of the new mineral devilliersite, $\text{Ca}_4\text{Ca}_2\text{Fe}^{3+}_{10}\text{O}_4[(\text{Fe}^{3+}_{10}\text{Si}_2)\text{O}_{36}]$

Biljana Krüger¹, Hannes Krüger¹, Irina O. Galuskina², Evgeny Galuskin², Yevgeny Vapnik³

¹University of Innsbruck, Innsbruck, Austria; ²University of Silesia, Sosnowiec, Poland; ³Ben-Gurion University of the Negev, Beer-Sheva, Israel; biljana.krueger@uibk.ac.at

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Poster - 45 Minerals-928-002_b.pdf

Formulation of clay refractory bricks: influence of the nature of chamotte and the alumina content in the clay

Moustapha SAWADOGO

Université Joseph KI ZERBO, Ouagadougou, Burkina Faso; sawtapha22@yahoo.fr

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Poster - 45 Minerals-717-003_b.pdf

Structural analysis of ilmenite concentrates treated by acid-assisted high energy ball milling

Tania Isabel Garcia-Manzano, José Antonio Henao-Martínez, Diana Marcela Cañas-Martínez, Julio Andres Pedraza-Avella
Universidad Industrial de Santander, Bucaramanga, Colombia; tania2188740@correo.uis.edu.co

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Poster - 45 Minerals-484-004_b.pdf

Investigation of structural phase transitions and superionic property of a Vanthoffite mineral, $\text{Na}_6\text{Co}(\text{SO}_4)_4$

Ajana Dutta, Diptikanta Swain, T. N. Guru Row

Indian Institute of Science, Bangalore, India, Bangalore, India; ajanadutta1@gmail.com

External Resource:



Poster - 45 Minerals-431-005_b.pdf

Raman, crystallographic and chemical characterization of roméite-group minerals.

Gerson Anderson de Carvalho Lopes¹, Daniel Atencio², Marcelo Barbosa de Andrade¹

¹São Carlos Institute of Physics, Av. Trabalhador São-carlense, 400, Pq. Arnold Schmidt – CEP 13566-590, São Carlos-SP - Brazil;

²Institute of Geosciences, Rua do Lago, 562, Butantã – CEP 05508-080, São Paulo-SP - Brazil; g.anderson@ifsc.usp.br

External Resource:



Poster - 45 Minerals-652-006_b.pdf

$\text{Cd}_4\text{Te}_5\text{O}_{14}$, consisting of $[\text{Te}_5\text{O}_{14}]$ -chains, a novel structure element for oxidotellurates(IV)

Felix Eder, Matthias Weil

TU Vienna, Vienna, Austria; felix.eder@tuwien.ac.at

External Resource:



Poster - 45 Minerals-1424-007_b.pdf



Poster - 45 Minerals-1424-007_c.pdf

Water induced variety of arsenic(III) oxide intercalates with alkali chlorides

Piotr A. Gunka

Warsaw University of Technology, Warszawa, Poland; piogun@ch.pw.edu.pl

External Resource:



Poster - 45 Minerals-695-008_b.pdf

Study of the NdO1.5-TiO2-ZrO2 ternary system of potential matrices for the immobilization of actinide wastes

Amina Sergeevna Ulanova, M S Nikolsky

IGEM, Moscow, Russian Federation; ulanova-amina@mail.ru

External Resource:



Poster - 45 Minerals-681-009_b.pdf

Ni₂MnGa shape memory alloy studied by x-ray diffraction measured in-situ in tension

Petr Cejpek¹, Kristián Mathis¹, Daria Drozdenko¹, Oleg Heczko², Ladislav Straka², Ross Colman¹

¹Charles University, Praha, Czech Republic; ²Institute of Physics of Czech Academy of Sciences, Praha, Czech Republic;
petr.cejpek@centrum.cz

External Resource:



Poster - 45 Minerals-812-010_b.pdf

⁵⁷Fe Mössbauer spectroscopy study of the Fe-bearing, Ge,Ga-rich synthetic tourmalines

Oxana Anosova¹, Kirill V. Frolov¹, Tatiana V. Setkova², Vladimir S. Balitsky², Elena Yu. Borovikova³

¹Shubnikov Institute of Crystallography of FSRC "Crystallography and Photonics" RAS, Moscow, Russian Federation; ²D.S. Korzhinskii Institute of Experimental Mineralogy RAS, Chernogolovka, Russian Federation; ³Faculty of Geology, Moscow State University, Moscow, Russian Federation; lm@crys.ras.ru

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Poster - 45 Minerals-1144-011_b.pdf

Co-crystal structure of a dinuclear (Zn-Y) and a trinuclear (Zn-Y-Zn) complexes derived from a Schiff base ligand

Ibrahima Elhadji Thiam¹, Mohamed Lamine Gaye¹, Javier Alcides Ellena², Mamour Sarr¹, Mayoro Diop¹, Natalia Alvarez³, Aliou Hamady Barry⁴

¹Université Cheikh Anta DIOP de Dakar, Dakar, Senegal; ²Instituto de Física de São Carlos, Universidade de São Paulo, CP 369, 13.560-970, São Carlos, SP, Brazil; ³Facultad de Química, General Flores 2124, UdelaR, Montevideo, 11800, Uruguay; ⁴Department of Chemistry, University of Nouakchott, Nouakchott, 130301, Mauritania; iethiam@yahoo.fr

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Poster - 45 Minerals-351-012_b.pdf

Copper(II) and zinc(II) complexes based on azo Schiff base ligand: Synthesis, crystal structure and photoisomerization study

Siham SLASSI¹, Abdelkrim EL-Ghayoury², Mohammed Aarjane¹, Amina Amine¹

¹Moulay Ismail University faculty of Science Meknes, Meknes, Morocco; ²Université d'Angers, France; Siham.slassi@gmail.com

External Resource:



Poster - 45 Minerals-325-013_b.pdf

Geopolymers based on some clay from Burkina Faso : preparation and characterization

Soungalo OUATTARA¹, Brahim SORGH¹, Lamine ZERBO¹, Youssouf SAWADOGO¹, Moustapha SAWADOGO¹, Mohamed SEYNOU¹, Philippe BLANCHART²

External Resource:



Poster - 45 Minerals-703-014_b.pdf

Impact of dopant type (Tm, Co, and Mn) and doping method on the local and statistical structure of framework whitlockite-type $\text{Ca}_3(\text{VO}_4)_2$ crystals. New crystal-chemical effects.

Galina Kuz'micheva¹, Irina Kaurova¹, Liudmila Ivleva²

¹MIREA - Russian Technological University, 78 Vernadsky ave., Moscow 119454, Russia; ²Prokhorov General Physics Institute, Russian Academy of Sciences, 38 Vavilova str., Moscow 119991, Russia; galina_kuzmicheva@list.ru

External Resource:



Poster - 45 Minerals-1419-015_b.pdf

Understanding the structure-property relationships of lead-free piezoelectric systems

Alicia Maria Manjon Sanz^{1,2}, Charles McLouth Culbertson², Caitlin Berger², Michelle Dolgos^{2,3}

¹Oak Ridge National Laboratory; ²Oregon State University; ³University of Calgary; manjonsanzam@ornl.gov

External Resource:



Poster - 45 Minerals-1462-016_b.pdf

New lead- and tellurium-free thermoelectric materials: $\text{AgSn}_m(\text{Sb}_x\text{Bi}_{1-x})\text{Se}_{m+2}$

Daniela Delgado¹, Paulina Valencia-Gálvez¹, María Luisa López², Inmaculada Álvarez-Serrano², Silvana Moris³, Antonio Galdámez¹

¹Departamento de Química, Facultad de Ciencias, Universidad de Chile, Las Palmeras 3425, Chile; ²Departamento de Química Inorgánica, Facultad de Ciencias Químicas, Universidad Complutense, 28040 Madrid; ³Centro de investigación de estudios avanzados del Maule (CIEAM), Vicerrectoría de Investigación y Postgrado, Universidad Católica del Maule, Avenida San Miguel 3605, Talca 3480112, Chile; dani.delgado.m@gmail.com

External Resource:



Poster - 45 Minerals-1516-017_b.pdf

What are the crystallographic and genetic implications of a naturally occurring polycrystal composed of two mineral phases of distinct symmetries and anionic groups? The case study of "joint-occurrence" of emerald+alexandrite polycrystals from Brazil

Teodoro Gauzzi¹, Leonardo Martins da Graça², Marco Antonio Leandro da Silva², Erico Tadeu Fraga Freitas¹, Breno Barbosa Moreira¹, Karla Balzuweit^{3,1}

¹Centro de Microscopia, Universidade Federal de Minas Gerais, Belo Horizonte, Brazil; ²Departamento de Geologia, Universidade Federal de Ouro Preto, Brazil; ³Departamento de Física, Universidade Federal de Minas Gerais, Brazil; karlaweit@gmail.com

External Resource:



Poster - 45 Minerals-1612-018_b.pdf

Effects upon Substitution in Alkali Metal Thallides: How far can X-Ray Structure Determination of Strongly Absorbing Compounds go?

Stefanie Gärtner

University of Regensburg, Institute of Inorganic Chemistry, Regensburg, Germany; stefanie.gaertner@ur.de

External Resource:



Poster - 45 Minerals-1342-019_b.pdf

Investigation of The Relationship between Groups and Subgroups in C3S's Structure Transition

dounia Tlamsamani, mbark ait mouha, khalid yamni

Materials, Molecular Engineering Environment Laboratory, Moulay Ismail University, Zitoun 11201, Morocco; douniayns@gmail.com

External Resource:



Poster - 45 Minerals-634-020_b.pdf

Synthesis and topotactic manipulation of layered oxysulfide $\text{CaSrMnO}_2\text{Cu}_{4-5}\text{S}_3$

Viktoria Falkowski, Simon J. Clarke

University of Oxford, Inorganic Chemistry Laboratory, South Parks Rd, Oxford, OX1 3QR, UK; viktoria.falkowski@chem.ox.ac.uk

External Resource:



Poster - 45 Minerals-1610-021_b.pdf

Ag, Cu, Hg, Pt, and Te substitutions in the synthetic analogue of palladseite, $\text{Pd}_{17}\text{Se}_{15}$: an experimental mineralogical study

František Laufek, Anna Vymazalová

Czech Geological Survey, Prague, Czech Republic; frantisek.laufek@geology.cz

External Resource:



Poster - 45 Minerals-1614-022_b.pdf

Charge density in fluorapatite, $\text{Ca}_5(\text{PO}_4)_3\text{F}$, from X-ray diffraction measurements on mineral and synthetic crystals

Agnieszka Huć¹, Marcin Stachowicz¹, D. E. Harlov², Jan Parafiniuk¹, Krzysztof Woźniak³

¹Institute of Geochemistry, Mineralogy and Petrology, Faculty of Geology, University of Warsaw, Żwirki i Wigury 93, Warsaw 02-089, Poland, Section 3.6; ²GeoForschungsZentrum, Telegrafenberg, 14473 Potsdam, Germany; ³Biological and Chemical Research Centre, Department of Chemistry, University of Warsaw, Żwirki i Wigury 101, Warszawa 02-093, Poland; a.huc@student.uw.edu.pl

External Resource:



Poster - 45 Minerals-1513-023_b.pdf

Crystal Chemistry, Phase Diagrams, and Thermoelectric Properties of the Ca-M-Co-O (M=Sr, La, Sm, Eu, Gd, and Ho) Systems

Winnie Wong-Ng¹, William Laws¹, Saul H Lapidus², Qing Huang¹, James A Kaduk^{3,4}

¹NIST, Gaithersburg, MD United States of America; ²APS, ANL, Argonne, IL United States of America; ³ITT, Chicago, IL United States of America; ⁴North Central College, Naperville, IL United States of America; winnie.wong-ng@nist.gov

External Resource:



Poster - 45 Minerals-1507-024_b.pdf

Crystal chemistry of halide containing silver borates.

Sergey Volkov¹, Dmitri Charkin², Manelis Lev², Rimma Bubnova¹

¹Grebenshchikov Institute of Silicate Chemistry, Saint-Petersburg, Russian Federation; ²Department of Chemistry, Lomonosov Moscow State University, Moscow, Russian Federation; s.n.volkov@inbox.ru

External Resource:



Poster - 45 Minerals-1687-026_b.pdf

Imidazole Based Ambiphilic Ligands for Anion Sensing, Metalation and Photophysical Properties

SABEEHA PARVEEN, AVINASH IRUTHAYARAJ, ANANTHARAMAN GANAPATHI

Indian Institute of Technology Kanpur, KANPUR, India; sabeeha@iitk.ac.in

External Resource:



Poster - 45 Minerals-1692-027_b.pdf

Phase structure of metallotermally reduced deep-sea concretion

Jaromír Kopeček¹, František Laufek², Alena Michalcová³, Lucie Šulcová³, Alisa Tsepeleva³, Eliška Chmelíková³, David Nováček³, Nguyen Hong Vu³, Petr Dvořák³, Pavel Novák³

¹FZU - Institute of Physics of the CAS, Praha, Czech Republic; ²Czech Geological survey, Praha, Czech Republic; ³University of Chemistry and Technology in Prague, Praha, Czech Republic; kopecek@fzu.cz

External Resource:





Poster - 45 Minerals-1874-028_b.pdf

Structural Landscape of Lanthanide coordinated Polyoxometalates

Shailabh Tewari, Arunachalam Ramanan

Indian Institute of Technology Delhi, Ghaziabad, India; shailabh.tewari@gmail.com

External Resource:



Poster - 45 Minerals-1689-029_b.pdf

Poster - 46 SAXS: SAXS, SANS

Session Chair: **Semra IDE**

Session Chair: **Jan Ilavsky**



5:10pm - 6:10pm

Poster session abstracts

Radomír Kužel



Poster - 46 SAXS-1973-001.pdf

Structural characterization of liposomes using integrated methods of HPLC/AF4, UV-Vis absorption, Refractive Index, MALLS, DLS, and SAXS

TingWei Hsu¹, Kuei-Fen Liao¹, Yi-Qi Yeh¹, Orion Shih¹, U-Ser Jeng^{1,2}

¹National Synchrotron Radiation Research Center, Hsinchu Science Park, Hsinchu 30076, Taiwan;; ²Department of Chemical Engineering, National Tsing Hua University, Hsinchu 30013;; myshine852@gmail.com

External Resource:



Poster - 46 SAXS-1320-002_b.pdf

Solution Structures of Intrinsically Disordered Dipeptide-Repeats Studied by SAXS and Molecular Structure Simulation

Tien-Chang Lin¹, U-Ser Jeng^{1,2}, Yun-Ru Chen³, Bing-Jun Lian¹, Kai-Tai Lin¹, Yu-Jen Chang³, Orion Shih², Yi-Qi Yeh², Kuei-Fen Liao²

¹Department of Chemical Engineering, National Tsing Hua University, Hsinchu 30013, Taiwan; ²National Synchrotron Radiation Research Center, Hsinchu, Taiwan; ³Genomics Research Center, Academia Sinica, 115, Taiwan

External Resource:



Poster - 46 SAXS-1288-003_b.pdf



Poster - 46 SAXS-1288-003_c.pdf

Nanostructural changes in commodity polyethylene during environmental exposure

Christopher Garvey^{1,2,3}, Ron Demjaha², Michael Weir⁴, Peter Halley⁵, Bronwyn Laycock⁵, Yu-Chieh Hsu⁵, Marianne Impéror-Clerc¹, Stéphan Rouzière¹

¹Technical University Munich, Garching, Germany; ²Lund Institute for Advanced Neutron and X-ray Science, 223 70 Lund, Sweden; ³Heinz Maier-Leibnitz Zentrum (MLZ), Lichtenbergstrasse 1 85747, Garching, Germany; ⁴School of Physics and Astronomy, University of Nottingham, University Park, Nottingham, NG7 2RD, United Kingdom; ⁵School of Chemical Engineering, The University of Queensland, St Lucia, Qld. 4067, Australia; christopher.garvey@tum.de

External Resource:



Poster - 46 SAXS-1205-004_b.pdf

Investigations of the precipitation microstructure in the alloys, hard metal composites, and powders using SANS

Vasyl Ryukhtin¹, Pavel Strunz¹, Ahmet Bahadır Yıldız², Pavel Zháňal^{3,4}, Kazuki Ohishi⁵, Yukihiko Kawamura⁵, Premysl Beran⁶, Snejana Bakardjieva⁷

¹Nuclear Physics Institute Řež, Řež, Czech Republic; ²Department of Materials Science and Engineering, KTH Royal Institute of Technology, SE-100 44 Stockholm, Sweden; ³Material and Mechanical Properties, Research Centre Řež Ltd., Řež, Czech Republic; ⁴Charles University in Prague, Faculty of Mathematics and Physics, Ke Karlovu 3, 12116, Prague, Czech Republic; ⁵Neutron Science and Technology Center, CROSS, Tokai, Ibaraki 319-1106, Japan; ⁶ESS AB, Lund, Sweden; ⁷Institute of Inorganic Chemistry CAS, 250 68 Husinec-Rez, Czech Republic; ryukhtin@ujf.cas.cz

External Resource:





Poster - 46 SAXS-1241-005_b.pdf

R&D Studies on metal oxide-based nanoparticles: Structure dependent physical and chemical properties

Gözde Bayazit Sekitmen¹, Rukiye Babaca Tosun¹, Süleyman Ali Tuncel², Semra İde³

¹Department of Nanotechnology and Nanomedicine, Hacettepe University, ANKARA, Turkey; ²Department of Chemical Engineering, Hacettepe University, ANKARA, Turkey; ³Department of Physics Engineering, Hacettepe University, ANKARA, Turkey; gozdebayazit@hacettepe.edu.tr

External Resource:



Poster - 46 SAXS-302-006_b.pdf



Poster - 46 SAXS-302-006_c.pdf

Revealing the Metal-Ligand Coordination effects on the Structure modifications for Balanced Tensile Modulus and Self-Healing of Polyurethane Films

Yu Sheng Lin¹, Chun-Hsiu Lin¹, Wei-Ru Wu², Chun-Jen Su², Ho-Hsiu Chou¹, An-Chung Su², U-Ser Jeng^{1,2}

¹National Tsing Hua University, Hsinchu, Taiwan; ²National Synchrotron Radiation Research Center, Hsinchu, Taiwan; stam86212@gmail.com

External Resource:



Poster - 46 SAXS-1292-007_b.pdf

Development of reference standard for small angle scattering measurement q calibration

R. Joseph Kline

NIST, Gaithersburg, United States of America; joe.kline@nist.gov

External Resource:



Poster - 46 SAXS-1318-008_b.pdf

Towards a better understanding of structure-performance relation in PEMFC fuel cells based on ptychography X-ray nanotomography and scanning small angle X-ray scattering

Christian Appel¹, Katharina Jeschonek², Kai Brunnengraber², Bastian Etzold², Marianne Liebi^{3,4}, Manuel Guizar-Sicairos¹

¹Paul Scherrer Institut, Villigen, Switzerland; ²Technische Universität Darmstadt, Darmstadt, Germany; ³EMPA, St. Gallen, Switzerland; ⁴Chalmers University of Technology, Gothenburg, Sweden; christian.appel@psi.ch

External Resource:



Poster - 46 SAXS-1550-009_b.pdf

Structural analysis of antibody complexes by inverse contrast-matching small-angle neutron scattering combined with size exclusion chromatography (SEC-ICM-SANS)

Nobuhiro Sato¹, Rina Yogo^{2,3,4}, Saeko Yanaka^{2,3,4}, Anne Martel⁵, Lionel Porcar⁵, Ken Morishima¹, Rintaro Inoue¹, Taiki Tominaga⁶, Takao Arimori⁷, Junichi Takagi⁷, Masaaki Sugiyama¹, Koichi Kato^{2,3,4}

¹Institute for Integrated Radiation and Nuclear Science, Kyoto University, Osaka, Japan; ²Institute for Molecular Science (IMS), National Institutes of Natural Sciences, Okazaki, Aichi, Japan; ³Exploratory Research Center on Life and Living Systems (ExCELLS), National Institutes of Natural Sciences, Okazaki, Aichi, Japan; ⁴Graduate School of Pharmaceutical Sciences, Nagoya City University, Nagoya, Aichi, Japan; ⁵Institut Laue-Langevin, Grenoble, France; ⁶Neutron Science and Technology Center, Comprehensive Research Organization for Science and Society (CROSS), Tokai, Ibaraki, Japan; ⁷Institute for Protein Research, Osaka University, Suita, Osaka, Japan

External Resource:



Poster - 46 SAXS-1529-010_b.pdf

Small-angle X-ray scattering beamlines at the photon factory

Nobutaka Shimizu¹, Hideaki Takagi¹, Yasuko Nagatani¹, Kento Yonezawa¹, Takeharu Mori¹, Keiko Yatabe¹, Masatsuyo Takahashi¹, Keishi Oyama¹, Noriyuki Igarashi¹

Institute of Materials Structure Science, High Energy Accelerator Research Organization (KEK), Tsukuba, Ibaraki, Japan; nobutaka.shimizu@kek.jp

External Resource:



Poster - 46 SAXS-1498-011_b.pdf

A pipeline for time-resolved small-angle X-ray scattering data analysis on amyloid fibrils formation in solution

Taja Cheremnykh¹, Mohsin Shafiq², Stefano Da Vela¹, Markus Glatzel², Dmitri Svergun¹

¹EMBL Hamburg, Hamburg, Germany; ²UKE, Hamburg, Germany; tcheremnykh@embl-hamburg.de

External Resource:  Presentation



Poster - 46 SAXS-1771-012_b.pdf

Poster - 47 Synchrotron and XFEL: Synchrotron and XFEL facilities

Session Chair: **Sofia Diaz-Moreno**

Session Chair: **Makina Yabashi**



5:10pm - 6:10pm

Poster session abstracts

Radomír Kužel



Poster - 47 Synchrotron and XFEL-1974-001.pdf

Beam heating from a fourth-generation synchrotron source

Eleanor Lawrence Bright, Carlotta Giacobbe, Jonathan Wright

European Synchrotron Radiation Facility, Grenoble, France; e.lawrencebright@esrf.fr

External Resource:  Presentation



Poster - 47 Synchrotron and XFEL-1275-002_b.pdf

Azimuthal integration and crystallographic algorithms on field-programmable gate arrays

Zdeněk Matěj¹, Kenneth Skovhede^{1,2}, Carl Johnsen², Artur Barczyk¹, Clemens Weninger¹, Andrii Salnikov¹, Brian Vinter²

¹MAX IV Laboratory, Lund University, Sweden; ²Niels Bohr Institute, University of Copenhagen, Denmark; zdenek.matej@maxiv.lu.se

External Resource:  Presentation



Poster - 47 Synchrotron and XFEL-1151-003_b.pdf

High-resolution synchrotron powder diffraction with the use of scanning 2D detector

Roman Svetogorov, Pavel Dorovatovskii, Vladimir Lazarenko

NRC Kurchatov Institute, Moscow, Russian Federation; rdsvetov@gmail.com

External Resource:  Presentation



Poster - 47 Synchrotron and XFEL-352-004_b.pdf

The APS upgrade: New Opportunities for Materials and Applied Science

Uta Ruett

Argonne National Laboratory, Lemont, United States of America; uruett@anl.gov

External Resource:  Presentation



Poster - 47 Synchrotron and XFEL-1654-005_b.pdf

Conceptual design of a scattering/diffraction beamline for the Russian synchrotron Ultimate Source for Synchrotron Radiation

Melanie Nentwich¹, Dmitri Novikov¹, Oliver Seeck¹, Timur V. Kulevoy², M. M. Borisov², Ilya A. Subbotin², Roman A. Senin²

¹DESY Photon Science, Hamburg, Germany; ²NRC "Kurchatov Institute" – Institute for Theoretical and Experimental Physics, Moscow, Russia; Melanie.Nentwich@desy.de

External Resource:  Presentation



Poster - 47 Synchrotron and XFEL-1460-006_b.pdf

The BioMAX beamline for macromolecular crystallography at MAX IV

Ana Gonzalez, **Oskar Aurelius**, Monika Bjelčić, Mikel Eguiraun, Ishkhan Gorgisyan, Elmir Jagudin, Sandesh Kanchugal, Tobias Krojer, Mirko Milas, Jie Nan, Thomas Ursby

MAX IV Laboratory, Lund, Sweden; oskar.aurelius@maxiv.lu.se

External Resource:



Poster - 47 Synchrotron and XFEL-1577-007_b.pdf

The Chemical Crystallography Beamline P24 - Status and Future Developments

Christian W. Lehmann¹, Christian Schäfer¹, Carsten Paulmann²

¹MPI für Kohlenforschung, Mülheim an der Ruhr, Germany; ²Universität Hamburg, Hamburg, Germany; lehmann@kofo.mpg.de

External Resource:



Poster - 47 Synchrotron and XFEL-1702-008_b.pdf

Possibilities at the Polar beamline at APS

Joerg Strempler, Steven Kearney, Altaf Khan, Daniela Capatina, Deming Shu, Ruben Reininger, Luca Rebuffi, Yongseong Choi, Gilberto Fabbris, Daniel Haskel

Argonne National Laboratory, Lemont, United States of America; strempler@anl.gov

External Resource:



Poster - 47 Synchrotron and XFEL-1682-009_b.pdf

KN-31: The contribution of crystallography to new vaccine formulations

Location: **Terrace 2A**

Session Chair: **Graciela Carlota Díaz de Delgado**

Marcia Fantini

Using crystallography tools to improve vaccine formulations

Márcia Carvalho de Abreu Fantini¹, Cristiano Luis Pinto Oliveira¹, José Luiz de Souza Lopes¹, Tereza da Silva Martins², Milena Apetito Akamatsu³, Aryene Góes Trezena⁴, Milene Tino de Franco⁴, Viviane Fongaro Botosso⁵, Osvaldo Augusto Brazil Esteves Sant'Anna⁶, Nikolay Kardjilov⁷, Martin Kjaerulf Rasmussen⁸, Heloísa Nunes Bordallo⁸

¹University of São Paulo, Physics Institute, São Paulo - SP, Brazil; ²Chemistry Department, Federal University of São Paulo, Diadema - SP, Brazil; ³Innovation Division, Butantan Institute, São Paulo - SP, Brazil; ⁴Imunogenetic Laboratory, Butantan Institute, São Paulo - SP, Brazil; ⁵Virology Laboratory, Butantan Institute, São Paulo - SP, Brazil; ⁶Imunochemistry Laboratory, Butantan Institute, São Paulo - SP, Brazil; ⁷HZB für Materialien und Energie, Helmholtz-Zentrum Berlin, Berlin, Germany; ⁸Niels Bohr Institute, University of Copenhagen.; mfantini@if.usp.br

External Resource:



KN-31-1572-001_b.pdf

KN-32: Crystallography and cultural heritage - On beauty, science and passion

Location: **Terrace 2B**

Session Chair: **Jose Miguel Delgado**

Gilberto Artioli

Crystallography and cultural heritage - On beauty, science and passion

Gilberto Artioli

Università di Padova, Padova, Italy; gilberto.artioli@unipd.it

External Resource:



KN-32-1576-001_b.pdf

KN-33: Overview of Global Neutron Sources, Instruments and Initiatives

Location: **Club A**

Session Chair: **Jiri Kulda**

Ken Andersen

Overview of Global Neutron Sources, Instruments and Initiatives

Ken Andersen

Oak Ridge National Laboratory, Oak Ridge, Tennessee, United States of America; andersenkh@ornl.gov

External Resource:



KN-33-1642-001_b.pdf

6:10pm - 7:00pm



6:10pm - 7:00pm



6:10pm - 7:00pm



8:00pm - 11:55pm

Dinner: Conference dinner

Location: **National House**
extra fee



Date: Saturday, 21/Aug/2021

9:00am - 9:50am

KN-34: Fabrication and Characterization of Inhomogeneity-free Polymer Gels

Location: **Club A**

Session Chair: **Marijana Đaković**

Mitsushiro Shibayama

Fabrication and characterization of inhomogeneity-free polymer gels

Mitsushiro Shibayama¹, Xiang Li², Yui Tsuji², Masato Ohira²

¹Comprehensive Research Organization for Science and Society, Tokai, Japan; ²The University of Tokyo, Kashiwa, Japan;
m_shibayama@cross.or.jp

External Resource: Presentation



KN-34-404-001_a.doc



KN-34-404-001_b.pdf



9:00am - 9:50am

KN-35: The Science of Symmetry Breaking

Location: **Terrace 2A**

Session Chair: **Oksana Zaharko**

Harold Stokes

The science of symmetry breaking: A personal journey

Harold T Stokes

Brigham Young University, Provo, United States of America; stokesh@byu.edu

External Resource: Presentation



KN-35-1224-001_b.pdf



9:00am - 9:50am

KN-36: Metadata and checkCIF for raw diffraction data in realising ultimate crystallographic objectivity

Location: **Terrace 2B**

Session Chair: **John Richard Helliwell**

Loes Kroon-Batenburg

Metadata and checkCIF for raw diffraction data and their role in realising crystallographic science objectivity

Loes M.J. Kroon-Batenburg

Utrecht University, Utrecht, The Netherlands; L.m.j.kroon-batenburg@uu.nl

External Resource: Presentation



KN-36-1569-001.doc



9:50am - 10:20am

Morning break 7: Coffee/tea

Location: **Exhibition and poster area**

MS-89: Fragment Screening, LCP, and Automation

Location: **Club B**

Session Chair: **Alice Douangamath**

Session Chair: **Lisa J. Keefe**

Invited: **Martin Noble (UK), Kenton Longenecker (USA)**

Introduction

10:20am - 10:25am

Introduction to session

Alice Douangamath, Lisa J. Keefe



MS-89-1819-001.pdf



10:20am - 12:45pm



10:25am - 10:55am

Fragment-Based Discovery of Orally Efficacious Allosteric Inhibitors of TNF-alpha

Kenton Longenecker

AbbVie, North Chicago, United States of America; kenton.longenecker@abbvie.com

External Resource: Presentation



10:55am - 11:25am

FragLites: a library of small molecules incorporating anomalous scatterers with applications in screening and protein interaction mapping

Martin E M Noble, Jane Endicott, Gemma Davison, Ian Hope, Mathew P Martin, Duncan Miller, Natalie Tatum, Max Temple, Shannon Turberville, James Sanderson, Dan Wood, Mike Waring
Newcastle University, Newcastle upon Tyne, United Kingdom



External Resource:



11:25am - 11:45am



Using sound pulses to solve the crystal harvesting bottleneck

Yasmin Samara¹, Haley Brennan², Liam McCarthy³, Mary Bollard⁴, Denise Laspina³, Jakub Wlodek⁵, Stefanie Campos⁶, Ramya Natarajan⁷, Kazimierz Gofron⁸, Sean McSweeney⁸, Alexei Soares⁸, Ludmila Leroy⁹

¹Universidade Federal de Santa Maria, 97105-900 Santa Maria-RS; ²Department of Biology, College of William and Mary, Williamsburg, VA 23187, USA; ³Department of Biology, Stony Brook University, New York, NY 11794-5215, USA; ⁴Department of Biology, York College of Pennsylvania, York, PA 17403, USA; ⁵Department of Computer Science, Stony Brook University, New York, NY 11794-5215, USA; ⁶Department of Clinical Nutrition, Stony Brook University, New York, NY 11794-5215, USA; ⁷Department of Biomedical Engineering, Georgia Institute of Technology, Atlanta, GA 30332, USA; ⁸Energy Sciences Directorate, NSLS II, Brookhaven National Laboratory, Upton, NY 11973-5000 USA; ⁹Universidade Federal de Minas Gerais, 31270-901 Belo Horizonte-MG, Brazil

External Resource:



MS-89-495-004_b.pdf

11:45am - 12:05pm



High throughput approach to prepare high-density microcrystals in lipidic cubic phase for serial crystallography and fragment screening

Isabel Moraes¹, Danny Axford², Agata Butryn², Pierre Aller², Tristan Kwan¹, Peter J Judge³

¹National Physical Laboratory, Teddington, UK; ²Diamond Light Source, Harwell Science and Innovation Campus, Didcot, OX11 0DE, UK; ³Biochemistry Department, University of Oxford, South Parks Road, Oxford, OX1 3QU, UK

External Resource:



MS-89-1031-005_b.pdf

12:05pm - 12:25pm



Fragment-based development of bacterial DsbA inhibitors as novel anti-virulence agents

Geging Wang¹, Wesam Alwan², Matthew Bentley², Biswaranjan Mohanty², Bradley Doak², Rabeb Dhouib³, Makrina Totsika³, Benvenuto Capuano², Peter Scammells², Jennifer Martin⁴, Martin Scanlon², Begoña Heras¹

¹Department of Biochemistry and Genetics, La Trobe Institute for Molecular Science, La Trobe University, Bundoora, VIC, 3086, Australia; ²Medicinal Chemistry, Monash Institute of Pharmaceutical Sciences, Monash University, Parkville, VIC, 3052, Australia; ³Institute of Health and Biomedical Innovation, Queensland University of Technology, Kelvin Grove, QLD, 4059; ⁴Griffith Institute for Drug Discovery, Griffith University, Nathan, QLD, 4111, Australia; g.wang@latrobe.edu.au

External Resource:



MS-89-1340-006_b.pdf

12:25pm - 12:45pm



Efficiently from Library to Hit – Crystallographic Fragment Screening in Berlin via Structurally Diverse Compound Libraries

Jan Wollenhaupt¹, Tatjana Barthel¹, Alexander Metz², Gustavo M.A. Lima³, Dirk Wallacher⁴, Elmir Jagudin³, Tobias Krojer³, Christian G. Feiler¹, Uwe Mueller¹, Gerhard Klebe², Manfred S. Weiss¹

¹Helmholtz-Zentrum Berlin, Macromolecular Crystallography; ²Philipps-Universität Marburg, Institute of Pharmaceutical Chemistry, Drug Design Group; ³MAX IV Laboratory, BioMAX; ⁴Helmholtz-Zentrum Berlin, Department Sample Environment

External Resource:



MS-89-864-007_b.pdf

MS-90: Structure solution and poorly crystalline materials



Location: **Terrace 2A**

Session Chair: **Angela Altomare**

Invited: **Martin Schmidt (Germany), Katharine Page (USA)**

Introduction

10:20am - 10:25am



Introduction to session

Angela Altomare



MS-90-1820-001.pdf

10:25am - 10:55am



Wrong organic crystal structures solved and refined from powder data

Martin U. Schmidt, Viktoria Gramakov, Carina Schlesinger, Lukas Tapmeyer

Goethe Universitaet, Frankfurt am Main, Germany; m.schmidt@chemie.uni-frankfurt.de

10:20am - 12:45pm

External Resource:



MS-90-622-002_b.pdf

10:55am - 11:25am

Probing Chemical Short-range Order and other Nanoscale Motifs in the Solid State

Katharine Page

University of Tennessee, Knoxville, United States of America; kpage10@utk.edu

External Resource:



MS-90-1300-003_b.pdf

11:25am - 11:45am

Multiscale structural decoding of fibrous materials by SAXS and WAXD

Antonia Neels, Alex Dommann, Anjani Maurya

Empa, Materials Science and Technology; antonia.neels@empa.ch

External Resource:



MS-90-926-004_b.pdf

11:45am - 12:05pm

Polarized resonant soft X-ray scattering measurements in polymer-grafted nanoparticles

Dean DeLongchamp

National Institute of Standards and Technology, Gaithersburg, United States of America; dean.delongchamp@nist.gov

External Resource:



MS-90-1309-005_b.pdf

12:05pm - 12:25pm

Understanding Order and Correlation in Liquid Crystals by Fluctuation Scattering

Jack Binns¹, Patick Adams¹, Cameron M. Kewish^{2,3}, Tamar L. Greaves¹, Andrew V. Martin¹

¹RMIT University, Melbourne, Australia; ²Australian Nuclear Science and Technology Organisation, Australian Synchrotron, Australia;

³La Trobe Institute for Molecular Science, La Trobe University, Australia; jack.binns@rmit.edu.au

External Resource:



MS-90-1034-006_b.pdf

12:25pm - 12:45pm

Using the Pair Angle Distribution Function for Analysing Protein Structure

Patrick Leslie Raphael Adams, Jack Binns, Tamar L. Greaves, Andrew V Martin

RMIT University, Melbourne, Australia; s3826109@student.rmit.edu.au

External Resource:



MS-90-1084-007_b.pdf

MS-91: Time-resolved phase evolution, interaction & crystallization in soft matter: Integrative approaches

Location: Club C

Session Chair: Mitsuhiro Shibayama

Session Chair: Jrjeng Ruan

Invited: Julia Kornfield (USA), Christine M. Papadakis (Germany)

Introduction

10:20am - 10:25am

Introduction to session

Mitsuhiro Shibayama, Jrjeng Ruan



MS-91-1821-001.pdf

10:25am - 10:55am

Metastable structures, interplay of sequential deformations, and interactions between tungsten disulfide nanotubes and poly(L-lactide) studied by *in situ* X-ray scattering

Julia Kornfield

Caltech, Pasadena, United States of America; jak@cheme.caltech.edu

External Resource:



[MS-91-1619-002_b.pdf](#)

10:55am - 11:25am

Kinetics of mesoglobule formation and disintegration in solutions of thermoresponsive polymers after fast pressure jumps

Christine Papadakis¹, Bart-Jan Niebuur¹, Leonardo Chiappisi², Florian A. Jung¹, Xiaohan Zhang¹, Alfons Schulte³

¹Technical University of Munich, Garching, Germany; ²Institut Laue-Langevin, Grenoble France; ³University of Central Florida, Orlando FL, U.S.A.; papadakis@tum.de

External Resource:



[MS-91-1392-003_b.pdf](#)

11:25am - 11:45am

Aggregation States and Proton Conductivity in Perfluorosulfonic Acid Thin Films under Humidity Condition

Daisuke Kawaguchi^{1,2}, Shigeki Yonemori¹, Yudai Ogata¹, Noboru Miyata³, Tessei Yoshida³, Tsukasa Miyazaki³, Hiroyuki Aoki^{4,5}, Keiji Tanaka^{1,2,6}

¹Department of Applied Chemistry, Kyushu University, Fukuoka, Japan; ²Center for Polymer Interface and Molecular Adhesion Science, Kyushu University, Japan; ³Neutron Science and Technology Center, Comprehensive Research Organization for Science and Society, Tokai, Japan; ⁴Materials and Life Science Division, J-PARC Center, Japan Atomic Energy Agency, Tokai, Japan; ⁵Institute of Materials Structure Science, High Energy Accelerator Research Organization, Tokai, Japan; ⁶International Institute for Carbon-Neutral Energy Research (WPI-I2CNER), Kyushu University, Fukuoka, Japan; d-kawaguchi@cstf.kyushu-u.ac.jp

External Resource:



[MS-91-1235-004_b.pdf](#)

11:45am - 12:05pm

Exploring the formation of Hf metal-organic frameworks

Francesca Catherine Firth¹, Michael Gaultois², Yue Wu², Joshua Stratford³, Dean Keeble⁴, Clare Grey¹, Matthew Cliffe⁵

¹Department of Chemistry, University of Cambridge, United Kingdom; ²Department of Chemistry, University of Liverpool, UK; ³School of Chemistry, University of Birmingham, UK; ⁴Diamond Light Source, Harwell Campus, UK; ⁵School of Chemistry, University of Nottingham, Nottingham, United Kingdom; fcnf2@cam.ac.uk

External Resource:



[MS-91-910-005_b.pdf](#)

12:05pm - 12:25pm

Transient Domain Structure of Coalescence-Induced Self-Organization in Droplet Phase Separation

Che-Min Chou¹, Wei-Tsung Chuang¹, Po-Da Hong²

¹National Synchrotron Radiation Research Center (NSRRC), Hsinchu, Taiwan; ²Department of Materials Science and Engineering, National Taiwan University of Science and Technology, Taipei, 10607, Taiwan; chou.cm@nsrrc.org.tw

External Resource:



[MS-91-1231-006_b.pdf](#)

12:25pm - 12:45pm

SAXS-revealed nanostructures of poly(ethylene glycol)-grafted phospholipid vesicles

Chun-jen Su

National Synchrotron Radiation Research Center, Hsinchu, Taiwan; su.cj@nsrrc.org.tw

External Resource:



[MS-91-1262-007_b.pdf](#)

10:20am - 12:45pm

MS-92 (34b): Structural biology of enzymes, mechanism and regulation II

Location: **Club A**

Session Chair: **Mirjam Czjzek**

10:20am - 10:50am

Structural insights into the transposition of antibiotic resistance

Georgy Smyshlyaev^{1,2,3}, Buse Isbilir^{1,2}, Carlos Rojas-Cordova^{1,2}, Anna Rubio-Cosials¹, Lotte Lambertsen¹, Alex Bateman³, Orsolya Barabas^{1,2}

¹University of Geneva, Geneva, Switzerland; ²Structural and Computational Biology Unit, European Molecular Biology Laboratory, Heidelberg, Germany; ³European Bioinformatics Institute, European Molecular Biology Laboratory, Hinxton, UK

External Resource:



MS-92 (34b)-1274-001_b.pdf

10:50am - 11:20am

Extraordinary Structures of Orphan Methyltransferases with Their Substrate DNA

John Horton, Jujun Zhou, Clayton Woodcock, Xing Zhang, Xiaodong Cheng

Department of Epigenetics and Molecular Carcinogenesis, The University of Texas -M.D. Anderson Cancer Center, Houston TX, USA

External Resource:



MS-92 (34b)-1360-002_b.pdf

11:20am - 11:40am

Structural and mechanistic basis for protein glutamylation by the kinase fold

Diana R. Tomchick¹, Miles H. Black¹, Adam Osinski¹, Krzysztof Pawlowski², Marcin Gradowski², Zhe Chen¹, Yang Li¹, Kelly A. Servage¹, Vincent S. Tagliabracci¹

¹UT Southwestern Medical Center, Dallas, United States of America; ²Warsaw University of Life Sciences, Warsaw, Poland

External Resource:



MS-92 (34b)-1313-003_b.pdf

11:40am - 12:00pm

Mechanism of RNA stimulated ATP hydrolysis by tick-borne encephalitis virus NS3 helicase

Paulina Duhita Anindita, Pavel Grinkevich, Marco Halbeisen, Roman Tuma, Zdenek Franta

Faculty of Science, University of South Bohemia, Ceske Budejovice, Czech Republic

External Resource:



MS-92 (34b)-847-004_b.pdf

12:00pm - 12:20pm

Quinol-dependent Nitric Oxide Reductases are dimers in cryoEM structures

Samar Hasnain

University of Liverpool, Liverpool, United Kingdom

External Resource:



MS-92 (34b)-165-005_b.pdf

12:20pm - 12:40pm

Interactive GUI for the calculation of Fobs-Fobs electron density difference maps and extrapolated structure factors based on the cctbx toolbox

Elke De Zitter¹, Nicolas Coquelle², Thomas Barends³, Jacques-Philippe Colletier¹

¹Institut de Biologie Structurale, Université de Grenoble Alpes, CEA, CNRS, 38044 Grenoble, France; ²Institut Laue-Langevin, 38044 Grenoble, France; ³Department of Biomolecular Mechanisms, Max Planck Institute for Medical Research, 69120 Heidelberg, Germany; elke.de-zitter@ibs.fr

External Resource:



MS-92 (34b)-1132-006_b.pdf

MS-93: Non-covalent interactions in crystal engineering I

Location: **Terrace 2B**

Session Chair: **Giuseppe Resnati**

Session Chair: **Petra Bombicz**

Invited: **Deepak Chopra** (India), **Karah Knope** (USA)

Introduction

10:20am - 10:25am

Introduction to session

Giuseppe Resnati, Petra Bombicz

10:20am - 12:45pm



MS-93-1822-001.pdf

10:25am - 10:55am

Understanding σ - and π -hole centered interactions in crystals from electron density analysis**Deepak Chopra**IISER Bhopal, Bhopal, India; dchopra@iiserb.ac.in

External Resource:



MS-93-175-002_b.pdf

10:55am - 11:25am

Harnessing non-covalent interactions towards the isolation of novel actinide structural units**Karah E Knope**Georgetown University, Washington, United States of America; kek44@georgetown.edu

External Resource:



MS-93-1323-003_b.pdf

11:25am - 11:45am

Stacking interactions of chelate rings of transition metal complexes**Dušan P. Malenov, Snežana D. Zarić**University of Belgrade - Faculty of Chemistry, Belgrade, Serbia; malenov@chem.bg.ac.rs

External Resource:



MS-93-500-004_b.pdf

11:45am - 12:05pm

Activating chalcogen bonding in alkylseleno/alkyltelluro acetylenes: Helical arrangements and crystal engineering strategies**Arun Dhaka¹, Olivier Jeannin¹, le-Rang Jeon¹, Emmanuel Aubert², Enrique Espinosa², Marc Fourmigué¹**¹Univ Rennes, CNRS, ISCR (Institut des Sciences Chimiques de Rennes) UMR 6226, 35042 Rennes; ²Laboratoire CRM2, UMR CNRS 7036, Institut Jean Barriol, Université de Lorraine, BP 70239, 54506 Vandœuvre-lès-Nancy; arun.dhaka@univ-rennes1.fr

External Resource:



MS-93-373-005_b.pdf

12:05pm - 12:25pm

Hydrogen bond architecture in a series of allylamine and normal alcohols (C₁-C₁₀) cocrystals.**Bernadeta Prus^{1,2}, Roland Boese¹, Michał Cyrański¹, Janusz Zachara², Łukasz Dobrzycki¹**¹University of Warsaw, Warsaw, Poland; ²Warsaw University of Technology, Warsaw, Poland; bernadeta.nowosielska@chem.uw.edu.pl

External Resource:



MS-93-470-006_b.pdf

12:25pm - 12:45pm

Expanding the crystal form landscape: emerging computational tools for the discovery of eutectic composites and higher-order cocrystals of organic compounds**Zeinab M. Saeed¹, Bhausheeb Dhokale¹, Abeer F. Shunnar¹, Durga P. Karothu², Pance Naumov², Hector H. Hernandez¹, Sharmarke Mohamed¹**¹Khalifa University of Science and Technology, Abu Dhabi, United Arab Emirates; ²New York University Abu Dhabi, Abu Dhabi, United Arab Emirates; sharmarke.mohamed@ku.ac.ae

External Resource:



MS-93-1019-007_b.pdf

10:20am - 12:45pm

MS-94: Organic minerals, metal-organic frameworks, and metal-oxygen clusters: the emergent interface of geochemistry and crystal engineering

Location: Club D

Session Chair: **Igor Huskić**
Session Chair: **Tomoji Ozeki**
Invited: **Helen Maynard-Casely (Australia), Ulrich Kortz (Germany)**

Introduction

10:20am - 10:25am

Introduction to session

Igor Huskić, Tomoji Ozeki



MS-94-1824-001.pdf

10:25am - 10:55am

Discrete polyoxometalates: from geochemistry via crystal engineering to functional materials

Ulrich Kortz

Jacobs University, Bremen, Germany; u.kortz@jacobs-university.de

External Resource:



MS-94-150-002_b.pdf

10:55am - 11:25am

Exploration of organic minerals on Saturn's moon Titan

Helen Maynard-Casely¹, Rob Hodyss², Tuan Vu², Michael Malaska², Mathieu Choukroun², Morgan Cable², Tom Runčevski³

¹Australian Nuclear Science and Technology Organisation, Kirrawee DC, Australia; ²NASA Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA, USA; ³Department of Chemistry, Southern Methodist University, Dallas, TX, USA; helenmc@ansto.gov.au

External Resource:



MS-94-720-003_b.pdf

11:25am - 11:45am

A Crystal Flask Composed of Huge Cage-of-Cage Metallosupramolecules for the Formation of Polyoxomolybdate

Tatsuhiro Kojima, Benny Wahyudianto, Takumi Konno

Osaka University, Osaka, Japan; kojimat15@chem.sci.osaka-u.ac.jp

External Resource:



MS-94-762-004_b.pdf

11:45am - 12:05pm

Autonomous Recombination and Selfhealing of Fracture in Piezoelectric Organic Crystals: Scopes in Crystal Engineering

Surojit Bhunia, Chilla Malla Reddy

Department of Chemical Sciences, Indian Institute of Science Education and Research (IISER) Kolkata, Kolkata, India; bhuniasurojit@gmail.com

External Resource:



MS-94-311-005_b.pdf

12:05pm - 12:25pm

Encapsulations of terpenes, aromatic and non-aromatic compound in metal-organic framework via the crystalline sponge method.

Faiza Habib, Derek Tocher, Claire Carmalt

University College London, London, United Kingdom; faiza.habib.17@ucl.ac.uk

External Resource:



MS-94-665-006_b.pdf

12:25pm - 12:45pm

Correlated Linker Disorder in Metal-Organic Frameworks

Emily Gabrielle Meekel

University of Oxford, Oxford, United Kingdom; emily.meekel@chem.ox.ac.uk

External Resource:





MS-94-411-007_b.pdf

MS-95: Advanced methods for analysis of XAFS and crystallographic data



Location: 223-4

Session Chair: **Marco Giorgetti**

Session Chair: **Paula Macarena Abdala**

Invited: **Paola D'angelo** (Italy), **Rocco Caliendo** (Italy)

Introduction

10:20am - 10:25am

Introduction to session

Marco Giorgetti, **Paula Macarena Abdala**



MS-95-1825-001.pdf

10:25am - 10:55am



Multivariate analysis of X-ray diffraction and XAFS data

Rocco Caliendo¹, **Annamaria Mazzone**¹, **Benny Danilo Belviso**¹, **Pietro Guccione**², **Marco Milanesio**³, **Luca Palin**³, **Mattia Lopresti**³

¹Institute of Crystallography, CNR, via Amendola 122/o, 70126, Italy; ²Dipartimento di Ingegneria Elettrica e dell'Informazione, Politecnico di Bari, via Orabona 4, Bari, 70125, Italy; ³Dipartimento di Scienze e Innovazione Tecnologica, Università del Piemonte Orientale, viale T. Michel 11, Alessandria, 15121, Italy; rocco.caliendo@ic.cnr.it

External Resource:



MS-95-946-002_b.pdf

10:55am - 11:25am



Advanced methods for the study of chemical systems by X-ray Absorption Spectroscopy

Paola D'Angelo

University of Rome La Sapienza, Rome, Italy; p.dangelo@uniroma1.it

External Resource:



MS-95-1648-003_b.pdf

11:25am - 11:45am



Analysis of XANES spectra for tektites using machine learning algorithms

Alexander Guda¹, **Sergey Guda**¹, **Andrea Martini**², **Antonina Kravtsova**¹, **Liubov Guda**¹, **Alexander Algasov**¹, **Alexander Soldatov**¹

¹The Smart Materials Research Institute, Southern Federal University, 344090 Rostov-on-Don, Russia; ²Department of Chemistry, INSTM Reference Center and NIS and CrisDi Interdepartmental Centers, University of Torino, 10125 Torino, Italy; guda@sfedu.ru

External Resource:



MS-95-614-004_b.pdf

11:45am - 12:05pm



Treatment of disorder effects in X-ray absorption spectra by reverse Monte-Carlo simulations: CuMoO₄ case

Inga Pudza, **Alexei Kuzmin**

Institute of Solid State Physics, University of Latvia, Riga, Latvia; inga.pudza@cfi.lu.lv

External Resource:



MS-95-1123-005_b.pdf

12:05pm - 12:25pm



Novel advanced methods in XAS – XERT and Hybrid Techniques

Christopher Thomas Chantler

University of Melbourne, Parkville, Australia; chantler@unimelb.edu.au

External Resource:



MS-95-427-006_b.pdf

Machine learning applied to operando XANES spectroscopy for Pd nanocatalysts

Oleg Usoltsev¹, Aram Bugaev^{1,2}, Alina Skorynina¹, Sergey Guda¹, Alexander Guda¹, Alexander Soldatov¹

¹The Smart Materials Research Institute of Southern Federal University; ²Federal State Budgetary Institution of Science "Federal Research Centre The Southern Scientific Centre of The Russian Academy of Sciences"; oleg-usol@yandex.ru

External Resource:



MS-95-185-007_b.pdf

MS-96: Crystallography schools to promote interdisciplinarity in science

Location: **Club H**

Session Chair: **Alice Brink**

Session Chair: **Serena Chiara Tarantino**

Invited: **Diego German Lamas (Argentina)**, **Marielle Yasmine Agbahoungbata (Benin)**

Introduction

10:20am - 10:25am

Introduction to session

Alice Brink, **Serena Chiara Tarantino**



MS-96-1826-001.pdf

10:25am - 10:55am

Crystallography schools and other educational activities in Latin America during the COVID-19 pandemic

Diego Germán Lamas

ITECA, UNSAM-CONICET, ECyT, Laboratorio de Cristalografía Aplicada, San Martín, Pcia. de Buenos Aires, Argentina; dlamas@unsam.edu.ar

External Resource:



MS-96-1178-002_b.pdf

10:55am - 11:25am

X-TechLab training sessions in Benin: towards borderless science education

Marielle Yasmine AGBAHOUNGBATA¹, **Sourou Albert Sidoine BONOU¹**, **Thierry d'ALMEIDA^{1,2}**, **Michele ZEMA³**, **Sekazi MTINGWA⁴**, **Claude BORNA¹**

¹Agence de Développement de Sèmè City, Cotonou, Benin; ²Commissariat à l'Energie Atomique et aux Energies Alternatives (CEA), France; ³University of Pavia, Italy; ⁴TriSEED Consultants, LLC, Hillsborough, NC, USA; hounmar@gmail.com

External Resource:



MS-96-1124-003_b.pdf

11:25am - 11:45am

Crystallographic education in real and reciprocal space

Dubravka Sisak Jung

DECTRIS, Baden-Daettwil, Switzerland; dubravka.sisak@dectris.com

External Resource:



MS-96-856-004_b.pdf

11:45am - 12:05pm

Teaching crystallographic symmetry in Latin America. A 10-year review and perspectives.

Leopoldo Suescun

Facultad de Química, Universidad de la República, Montevideo, Uruguay; leopoldo@fq.edu.uy

External Resource:



MS-96-953-005_b.pdf

12:05pm - 12:25pm

High impact crystallography skills development through local undergraduate curriculum and regional workshops and schools

Louise Nicole Dawe

Wilfrid Laurier University, Waterloo, Canada; ldawe@wlu.ca

External Resource:





MS-96-884-006_b.pdf

12:25pm - 12:45pm

Crystallography for all – Using the CSD to help promote interdisciplinarity in science

Suzanna Ward, **Ilaria Gimondi**

The Cambridge Crystallographic Data Centre (CCDC), Cambridge, United Kingdom; ward@ccdc.cam.ac.uk

External Resource:



MS-96-1570-007_b.pdf

SMS-7: Hydrogen rich compounds: design, properties & phase transitions at high pressures

Location: **221-2**

Session Chair: **Artem R Oganov**

Session Chair: **Alexander Goncharov**

Invited: **Chris J. Pickard (UK)**, **Dmitry Semenok (Russia)**

Introduction

10:20am - 10:25am

Introduction to session

Artem R Oganov, **Alexander Goncharov**



SMS-7-1841-001.pdf

10:25am - 10:55am

Computational challenges in the search for better superconducting hydrides

Christopher James Pickard

University of Cambridge, Cambridge, United Kingdom; cjp20@cam.ac.uk

External Resource:



SMS-7-1010-002_b.pdf

10:55am - 11:25am

Room-temperature superconductivity in compressed polyhydrides

Dmitrii Semenok

Skolkovo Institute of Science and Technology, Moscow, Russian Federation; dmitrii.semenok@skoltech.ru

External Resource:



SMS-7-633-003_b.pdf

11:25am - 11:55am

Electronegativity and Mendeleev number: redefinition of two important atomic chemical descriptors

Artem R Oganov

Skoltech, Moscow, Russian Federation; a.oganov@skoltech.ru

External Resource:



SMS-7-1664-004_b.pdf

12:45pm - 2:45pm

Lunch 7: Lunches

Location: **Exhibition and poster area**

MS-100: Stimuli-responsive crystalline compounds

Location: **Club B**

Session Chair: **Chiara Massera**

Session Chair: **Ivan Halasz**

Invited: **Tomce Runcevski (USA)**, **Helena Shepherd (UK)**

Introduction

2:45pm - 2:50pm

Introduction to session

Chiara Massera, **Ivan Halasz**



MS-100-1827-001.pdf

2:50pm - 3:20pm

Structural Insights into the Temperature-induced Color Changes of $[(CH_3)_2NH_2]_2NiCl_4$



Tomce Runcevski

Southern Methodist University, Dallas, United States of America; truncovski@smu.edu

External Resource:



MS-100-718-002_b.pdf

3:20pm - 3:50pm



Smart Molecular Materials: Synthesis, Structure and Properties

Helena Shepherd

University of Kent, Canterbury, United Kingdom; h.j.shepherd@kent.ac.uk

External Resource:



MS-100-1052-003_b.pdf

3:50pm - 4:10pm



Ultra-Fast Rotors and Light Emitting Ligands in Metal-Organic Frameworks

Angiolina Comotti, Silvia Bracco, Jacopo Perego, Charl X. Bezuidenhout, Sergio Piva, Piero Sozzani

University of Milano Bicocca, Milano, Italy; angiolina.comotti@unimib.it

External Resource:



MS-100-756-004_b.pdf

4:10pm - 4:30pm



Shape-memory effects in molecular crystals

Ejaz Ahmed¹, Durga Prasad Karothu¹, Mark Warren², Pance Naumov¹

¹New York University, Abu Dhabi, United Arab Emirates; ²Diamond Light Source, Didcot, Oxfordshire, OX11 0DE, United Kingdom; ea79@nyu.edu

External Resource:



MS-100-160-005_b.pdf

4:30pm - 4:50pm



Low-power photo-carving of dye-volatile cocrystals: The sublime cutting edge of light-responsive materials

Tristan Hermann Borchers, Filip Topic, Tomislav Friščić, Christopher John Barrett

McGill University, Montréal, Canada; tristan.borchers@mail.mcgill.ca

External Resource:



MS-100-1156-006_b.pdf

4:50pm - 5:10pm



Crystal locomotion driven by photo-triggered phase transition

Yuki Hagiwara¹, Akifumi Takanabe¹, Toru Asahi^{1,2}, Hideko Koshima²

¹Graduate school of Advanced Science and Engineering, Waseda University, Tokyo, Japan; ²Research Organization for Nano & Life Innovation, Waseda University, Tokyo, Japan; miller-yh0514@fuji.waseda.jp

External Resource:



MS-100-1252-007_b.pdf

MS-101 (18b): Phase transitions in complex materials (structure and magnetism) II



Location: Club A

Session Chair: Yuichi Shimakawa

Session Chair: Alexandra Gibbs

2:45pm - 5:10pm

2:45pm - 3:05pm



Towards an iterative exploration of novel materials exhibiting electronic phase transitions

James M. Rondinelli

Northwestern University, Evanston, United States of America; jrondinelli@northwestern.edu

External Resource:





MS-101 (18b)-1130-001_b.pdf

3:05pm - 3:25pm

Negative X-ray expansion in cadmium cyanide

Chloe Simone Coates^{1,2}, Claire A. Murray³, Hanna L. B. Bostrom⁴, Emily M. Reynolds⁵, Andrew L. Goodwin²

¹Department of Chemistry, Cambridge, U. K, CB2 1EW; ²Inorganic Chemistry Laboratory, Oxford, U. K., OX1 3QR; ³Diamond Light Source, Didcot, Oxfordshire OX11 0DE, U. K; ⁴Nanochemistry Department, Max Planck Institute for Solid State Research, Stuttgart, Germany, 70569; ⁵ISIS Facility, Didcot, Oxfordshire, U. K., OX11 0QX; cc2084@cam.ac.uk

External Resource:



MS-101 (18b)-950-002_b.pdf

3:25pm - 3:45pm

Crystal structure, complex phase diagram and re-entrant phase transition in NaSrPO₄

Gwilherm Nénert

Malvern Panalytical, Almelo, Netherlands, The; gwilherm.nenert@malvernpanalytical.com

External Resource:



MS-101 (18b)-924-003_b.pdf

3:45pm - 4:05pm

Crystal structure of a new polymorph of Sr₂TiO₄ with tetrahedral titanium

Dorota Pulmannova, Céline Besnard, Enrico Giannini

University of Geneva, Quai Ernest-Ansermet 24, 1205 Geneva, Switzerland; dorota.pulmannova@unige.ch

External Resource:



MS-101 (18b)-1030-004_b.pdf

4:05pm - 4:25pm

Revisiting the crystal structure and magneto-elastic coupling in MnZnSb

Kieran Jon Routledge¹, Philip A.E. Murgatroyd¹, John B. Claridge², Stanislav N. Savvin³, Jonathan Alaria¹

¹Department of Physics, University of Liverpool, United Kingdom; ²Department of Chemistry, University of Liverpool, United Kingdom;

³Institut Laue-Langevin, France; K.Routledge@liverpool.ac.uk

External Resource:



MS-101 (18b)-1110-005_b.pdf

4:25pm - 4:45pm

Phase transitions and magnetic structures in Epsilon-Fe₂O₃ nanoparticles

Arnau Romaguera¹, Zheng Ma¹, Javier Herrero-Martín², Catalin Popescu², Juan Angel Sans³, Martí Gich¹, Jose Luis Garcia-Muñoz¹

¹Institut de Ciència de Materials de Barcelona, ICMAB-CSIC, Bellaterra, Spain; ²CELLS-ALBA synchrotron, Cerdanyola del Vallès, Spain; ³Instituto de Diseño para la Fabricación, Universitat Politècnica de València, Valencia, Spain; aromaguera@icmab.es

External Resource:



MS-101 (18b)-934-006_b.pdf

4:45pm - 5:05pm

Polytypism in layered AB₂ solids

Emma Helen Wolpert¹, Andrew L Goodwin²

¹Department of Chemistry, Imperial College London, London, United Kingdom; ²Inorganic Chemistry, University of Oxford, Oxford, United Kingdom; e.wolpert@imperial.ac.uk

External Resource:



MS-101 (18b)-918-007_b.pdf

2:45pm - 5:10pm

MS-102: Crystallography using large volume presses and diamond anvil cells

Location: Terrace 2B



Session Chair: **Shanti Deemyad**
Session Chair: **Ronald MILETICH**
Invited: **Natalia Dubrovinskaia (Germany), Siddharth Saxena (UK)**

Introduction

2:45pm - 2:50pm

Introduction to session

Shanti Deemyad, Ronald Miletich



MS-102-1828-001.pdf

2:50pm - 3:20pm

Evolution of Structural, Magnetic and Electronic Properties with Pressure in TMPX_3 van-der-Waals Compounds

Siddharth Saxena

University of Cambridge, United Kingdom (Gb), United Kingdom; sss21@cam.ac.uk

External Resource:



MS-102-1177-002_b.pdf

3:20pm - 3:50pm

Materials synthesis and crystallography at extreme pressure-temperature conditions

Natalia Dubrovinskaia¹, Leonid Dubrovinsky²

¹Laboratory of Crystallography, Universität Bayreuth, Bayreuth, Germany; ²Bayerisches Geoinstitut, Universität Bayreuth, Bayreuth, Germany; Natalia.Dubrovinskaia@uni-bayreuth.de

External Resource:



MS-102-1631-003_b.pdf

3:50pm - 4:10pm

Salts of guanine and alkali metals: preparation and structural study at broad range of T, P

Anna Gaidamaka^{1,2}, Sergey Arkhipov^{1,2}, Boris Zakharov^{1,2}, Yuri Seryotkin^{1,3}, Elena Boldyreva^{1,2}

¹Novosibirsk State University, Novosibirsk, Russian Federation; ²Borisev Institute of Catalysis SB RAS, Novosibirsk, Russian Federation; ³V.S. Sobolev Institute of Geology and Mineralogy SB RAS, Novosibirsk, Russian Federation; a.gaidamaka@ng.su.ru

External Resource:



MS-102-371-004_b.pdf

4:10pm - 4:30pm

Phase diagram of carbon dioxide revisited

Kamil Filip Dziubek¹, Demetrio Scelta^{1,2}, Martin Ende³, Ronald Miletich³, Roberto Bini^{1,2,4}, Mohamed Mezouar⁵, Gaston Garbarino⁵

¹LENS - European Laboratory for Non-Linear Spectroscopy, Sesto Fiorentino, Italy; ²ICCOM-CNR, National Research Council of Italy, Sesto Fiorentino, Italy; ³Institut für Mineralogie und Kristallographie, Universität Wien, Wien, Austria; ⁴Dipartimento di Chimica "Ugo Schiff" dell'Università degli Studi di Firenze, Sesto Fiorentino, Italy; ⁵European Synchrotron Radiation Facility, ESRF, Grenoble, France; dziubek@lens.unifi.it

External Resource:



MS-102-959-005_b.pdf

4:30pm - 4:50pm

X-ray study of krypton and xenon under pressure reveals the mechanism of martensitic transformations

Angelika Dorothea Rosa¹, Agnes Dewaele², Gaston Garbarino¹, Irifune Tetsuo³, Olivier Mathon¹, Mohamed Ali Bouhifd⁴

¹ESRF, Grenoble, France; ²CEA, Arpajon Cedex, France; ³Geodynamics Research Center, Ehime University, Matsuyama, Japan; ⁴9. Laboratoire Magmas et Volcans, Université Clermont Auvergne, Clermont-Ferrand, France; arosa@esrf.fr

External Resource:



MS-102-768-006_b.pdf

2:45pm - 5:10pm

MS-103: XAS and crystallography allied for geomaterials and environmental problems

Location: 223-4

Session Chair: **J. Fred Mosselmans**

Session Chair: **Annalisa Martucci**

Invited: **Giuseppe Cruciani (Italy), Georgia Cametti (Switzerland)**



Introduction

2:45pm - 2:50pm

Introduction to session

J. Fred Mosselmans, Annalisa Martucci



MS-103-1829-001.pdf

2:50pm - 3:20pm

Immobilization and removal of hazardous elements by geomaterials: the harder and the softer solutions

Giuseppe Cruciani

University of Ferrara, Ferrara, Italy; gru@unife.it

External Resource:



MS-103-1382-002_b.pdf

3:20pm - 3:50pm

Combining X-ray diffraction, X-ray absorption spectroscopy, and molecular dynamics simulations to probe metals in zeolites: the case of intergrown Cd^{2+} -LEV/ERI

Georgia Cametti¹, Andreas C. Scheinost^{2,3}, Sergey V. Churakov^{1,4}

¹Bern Universität, Bern, Switzerland; ²The Rossendorf Beamline at the European Synchrotron Radiation Facility (ESRF), Avenue des Martyrs 71, 38043 Grenoble, France; ³Helmholtz Zentrum Dresden Rossendorf, Institute of Resource Ecology, Bautzner Landstrasse 400, 01328, Dresden, Germany; ⁴Paul Scherrer Institut, Forschungstrasse 111, 5232, Villigen PSI, Switzerland; georgia.cametti@geo.unibe.ch

External Resource:



MS-103-899-003_b.pdf

3:50pm - 4:10pm

Adsorption and degradation mechanisms of perfluoroalkyl substances (PFAS) on Ag-exchanged FAU-type zeolite studied by in situ synchrotron X-ray diffraction and thermal analysis/isotope ratio mass spectrometry.

Maura Mancinelli¹, Lara Gigli², Matteo Ardit¹, Jasper Rikkert Plaisier², Gianluca Bianchini¹, Gian Marco Salani¹, Annalisa Martucci¹

¹Department of Physics and Earth Sciences, University of Ferrara, Via Saragat 1, I-44121, Ferrara, Italy; ²Elettra-Sincrotrone Trieste S.C.p.A., Materials Characterisation By X-ray diffraction (MCX) Beamline, Strada Statale 14 - km 163,5 in AREA Science Park, Basovizza, Trieste, Italy; mncmra1@unife.it

External Resource:



MS-103-917-004_b.pdf

4:10pm - 4:30pm

Revealing the lifelong bio-persistent crystal structure of an asbestos fibre

Carlotta Giacobbe¹, Dario Di Giuseppe^{2,3}, Alessandro Zoboli², Paola Bonasoni⁴, Anna Moliterni⁵, Jonathan Wright¹, Alessandro Gualtieri²

¹aEuropean Synchrotron Radiation Facility, 71, Avenue Des Martyrs, Grenoble, 38040, France; ²bDepartment of Chemical and Geological Sciences, University of Modena and Reggio Emilia, Modena, 41121, Italy; ³cDepartment of Sciences and Methods for Engineering, University of Modena and Reggio Emilia, Via Amendola, 2, Reggio Emilia, 42122, Italy; ⁴Pathology Unit, Azienda Unità Sanitaria Locale - IRCCS, Reggio Emilia, Italy; ⁵Istituto di Cristallografia, CNR, Via Amendola, 122/o, Bari, 70126, Italy; carlotta.giacobbe@esrf.fr

External Resource:



MS-103-1261-005_b.pdf

4:30pm - 4:50pm

Mechanisms of structural reordering during thermal transformation of aluminogermanate imogolite nanotubes

Geoffrey Monet¹, Stéphan Rouzière¹, Delphine Vantelon², Pascale Launois¹, Erwan Paineau¹

¹Laboratoire de Physique des Solides, CNRS, université Paris-Saclay, Orsay, France; ²Synchrotron SOLEIL, Saint-Aubin, France; pascale.launois@universite-paris-saclay.fr

External Resource:



MS-103-783-006_b.pdf

4:50pm - 5:10pm

Evolution of the wall-crystal interface as witness of the heterogeneous nucleation and growth of Naica's giant crystals

Maria Elena Montero-Cabrera¹, Bernardo Pérez-Cázares², María Elena Fuentes-Montero², Luis Edmundo Fuentes-Cobas¹, Isai Castillo-Sandoval¹, Iván Jalil Carreño-Márquez³, Hilda Esperanza Esparza-Ponce¹, Diane Eichert⁴, René Loredó-Portales⁵, Lorena Pardo⁶

¹Centro de Investigación en Materiales Avanzados, Chihuahua, Mexico; ²Universidad Autónoma de Chihuahua, Chihuahua, Mexico; ³Universidad La Salle Chihuahua, Chihuahua, Mexico; ⁴Elettra Sincrotrone-Trieste, Basovizza, Italy; ⁵CONACYT-Universidad nacional Autónoma de México, Hermosillo, Mexico; ⁶Instituto de Ciencia de Materiales de Madrid, Madrid, Spain; rloredop@geologia.unam.mx

External Resource:



MS-103-1221-007_b.pdf

MS-104: Diffraction imaging, grain mapping in materials and art



Location: **Terrace 2A**

Session Chair: **Jonathan Paul Wright**

Session Chair: **Sine Larsen**

Invited: **Ashley Bucsek (USA)**, **Frederik Vanmeert (Belgium)**

Introduction

2:45pm - 2:50pm

Introduction to session

Jonathan Paul Wright, Sine Larsen



MS-104-1830-001.pdf

2:50pm - 3:20pm

Macroscopic X-ray powder diffraction imaging for the study of oil paintings



Frederik Vanmeert^{1,2}, Steven de Meyer¹, Arthur Gestels¹, Steven Saverwyns², Koen Janssens¹

¹AXES Research Group, NANOLab Centre of Excellence, University of Antwerp, Antwerp, Belgium; ²Laboratory Department, Royal Institute for Cultural Heritage, Brussels, Belgium; frederik.vanmeert@uantwerpen.be

External Resource:



MS-104-1345-002_b.pdf

3:20pm - 3:50pm

A multiscale, multimodal approach to studying static recrystallization in Mg-3Zn-0.1Ca



Sangwon Lee¹, Tracy Berman¹, Can Yildirim², Kate Shanks³, Carsten Detlefs², John Allison¹, Ashley Bucsek¹

¹University of Michigan, Ann Arbor, United States of America; ²European Synchrotron Radiation Facility, Grenoble, France; ³Cornell High Energy Synchrotron Source, Ithaca, United States of America; abucsek@umich.edu

External Resource:



MS-104-1437-003_b.pdf

3:50pm - 4:10pm

Trindex - 3D Grain Orientation Mapping with Neutron Imaging



Patrick Kin Man Tung¹, Stavros Samothrakitis², Camilla Larsen², Nancy Elewa³, Ryoji Kiyanagi⁴, Takenao Shinohara⁴, Luise Theil Kuhn⁵, Robin Woracek⁶, Markus Strobl², Petr Sittner³, Soren Schmidt⁶

¹University of New South Wales, Australia; ²Paul-Scherrer Institute, Switzerland; ³Institute of Physics, Czech Republic; ⁴Japan Proton Accelerator Research Complex (J-PARC), Japan; ⁵Technical University of Denmark, Denmark; ⁶European Spallation Source ERIC, Sweden; patrick.tung@unsw.edu.au

External Resource:



MS-104-886-004_b.pdf

4:10pm - 4:30pm

New advanced tools for processing and analysis of 2D X-ray diffraction data: XRD2DScan software 7.0



Alejandro Rodríguez-Navarro¹, Natalia Dadivanyan², Anil Kumar², Milen Gateshki²

¹Universidad de Granada, 18002 Granada, Spain; ²Malvern Panalytical B.V., 7602 EA Almelo, The Netherlands; anava@ugr.es

External Resource:



MS-104-861-005_b.pdf

4:30pm - 4:50pm

Visualizing the Dynamics of Subsurface Defects with Time-Resolved Dark-Field X-ray Microscopy



Leora Dresselhaus-Marais
Lawrence Livermore National Lab, Livermore, United States of America; leoradm@stanford.edu

External Resource:  Presentation



[MS-104-1239-006_b.pdf](#)

4:50pm - 5:10pm



Diffraction imaging and tomography investigations on the hydration of gypsum plaster

Michela La Bella^{1,2}, Rogier Besselink², Alexander E. S. Van Driessche², Jonathan P. Wright¹, Carlotta Giacobbe¹, Alejandro Fernandez-Martinez²

¹European Synchrotron Radiation Facility, 71 Avenue Des Martyrs, 38040 Grenoble, France; ²Institut de science de la Terre, Université Grenoble Alpes, 1381 Rue de la Piscine, 38610 Gières, France; michela.la-bella@esrf.fr

External Resource:  Presentation



[MS-104-1218-007_b.pdf](#)

MS-97: New methods to fight the pandemic



Location: **Panorama**

Session Chair: **Jane Shelby Richardson**

Session Chair: **Nicholas Mark Pearce**

Invited: **Jasmine Young (USA), Tristan Croll (UK)**

Introduction

2:45pm - 2:50pm



Introduction to session

Jane Shelby Richardson, Nicholas Mark Pearce



[MS-97-1831-001.pdf](#)

2:50pm - 3:20pm



"Enhanced peer review" - rebuilding early SARS-CoV-2 structures in ISOLDE

Tristan Ian Croll

University of Cambridge, Cambridge, United Kingdom

External Resource:  Presentation



[MS-97-1348-002_b.pdf](#)

3:20pm - 3:50pm



Improving the quality of 3D structure data in the Protein Data Bank with coordinate versioning supported by OneDep

Jasmine Y. Young

RCSB Protein Data Bank, Institute for Quantitative Biomedicine, Rutgers, The State University of New Jersey, Piscataway, United States of America

External Resource:  Presentation



[MS-97-1033-003_b.pdf](#)

3:50pm - 4:15pm



Neutron crystallography for drug design targeting SARS-CoV-2 viral proteins

Andrey Kovalevsky, Daniel Kneller, Leighton Coates

Oak Ridge National Lab, Oak Ridge, United States of America

External Resource:  Presentation



[MS-97-1000-004_b.pdf](#)

4:15pm - 4:40pm



The temperature-dependent conformational ensemble of SARS-CoV-2 main protease (M^{Pro})

Ali Ebrahim^{1,2}, Blake T. Riley², Desigan Kumaran³, Babak Andi^{4,5}, Martin R. Fuchs⁴, Sean McSweeney^{4,5}, Daniel A. Keedy^{2,6,7}

¹Diamond Light Source, Harwell Science and Innovation Campus, Didcot OX11 0DE, England; ²Structural Biology Initiative, CUNY Advanced Science Research Center, New York, NY 10031; ³Biology Department, Brookhaven National Laboratory, Upton, NY 11973; ⁴National Synchrotron Light Source II, Brookhaven National Laboratory, Upton, NY 11973; ⁵National Virtual Biotechnology Laboratory (NVBL), US Department of Energy, Washington, DC, United States; ⁶Department of Chemistry and Biochemistry, City College of New York, New York, NY 10031; ⁷Ph.D. Programs in Biochemistry, Biology, and Chemistry, The Graduate Center – City University of New York, New York, NY 10016

External Resource:



MS-97-1207-005_b.pdf

4:40pm - 5:05pm

Validation of cryo-EM structures of SARS-CoV-2 and mapping genomic mutations

Agnel Praveen Joseph, Sony Malhotra, Martyn Winn

STFC, Scientific Computing Department, Harwell, Didcot, United Kingdom

External Resource:



MS-97-1227-006_b.pdf

MS-98: 2D type crystals and their heterostructures

Location: **Club C**

Session Chair: **Matteo Bosi**

Session Chair: **Adela Rodríguez-Romero**

Invited: **Eli Sutter (USA)**, Xinliang Feng (Germany)

Introduction

2:45pm - 2:50pm

Introduction to session

Matteo Bosi, **Adela Rodríguez-Romero**



MS-98-1832-001.pdf

2:50pm - 3:20pm

1D Nanowires of 2D Layered Materials: A New Frontier in Nanomaterials

Eli Sutter, **Peter Sutter**

University of Nebraska-Lincoln, Lincoln, United States of America; esutter@unl.edu

External Resource:



MS-98-705-002_b.pdf

3:20pm - 3:50pm

Advances in organic 2D crystals

Xinliang Feng

Technische Universität Dresden, Dresden, Germany; xinliang.feng@tu-dresden.de

External Resource:



MS-98-1676-003_b.pdf

3:50pm - 4:10pm

Crystal growth and characterisation of organic-inorganic lead-free 2D double perovskite for application in radiation sensin

Valeria Murgulov¹, Catherine Schweinle², Michael Daub^{1,2}, Harald Hillebrecht^{1,2}, Michael Fiederle¹

¹Freiburg Materials Research Center FMF, Albert-Ludwigs-Universität Freiburg, Germany; ²Institute of Inorganic and Analytical Chemistry, Faculty of Chemistry and Pharmacy, Albert-Ludwigs-Universität Freiburg, Germany; valeria.murgulov@fmf.uni-freiburg.de

External Resource:



MS-98-794-004_b.pdf

4:10pm - 4:30pm

Determination of stress, cracks and defects density in crystals after wafer-bonding processes: a novel HRXRD – X-ray micro CT conjoint analytical approach

Aurelio Borzi¹, Robert Zboray¹, Simone Dolabella^{1,2}, Alex Dommann¹, Antonia Neels^{1,2}

¹Center for X-ray Analytics, Empa, Ueberlandstrasse 129, Dübendorf, Switzerland; ²Department of Chemistry, University of Fribourg, Avenue de l'Europe 20, 1700 Fribourg, Switzerland; aurelio.borzi@empa.ch

External Resource:



MS-98-801-005_b.pdf

2:45pm - 5:10pm

4:30pm - 4:50pm

Crystallography online by the Bilbao Crystallographic Server: new computer tools for the study of layer and multi-layer materials

Gemma de la Flor¹, Emre Tasci², Luis Elcoro³, Gotzon Madriaga³, Juan Manuel Perez-Mato³, Yuri E. Kitaev⁴, Robert Evarestov⁵, Mois I. Aroyo³

¹Institute of Applied Geosciences, Karlsruhe Institute of Technology, Karlsruhe, Germany; ²Department of Physics Engineering, Hacettepe University, Ankara, Turkey; ³Departamento de Física de la Materia Condensada, Universidad del País Vasco UPV/EHU, Leioa, Spain; ⁴Laboratory of Quantum-size Heterostructures, Ioffe Institute, Saint Petersburg, Russia; ⁵Institute of Chemistry, Saint Petersburg State University, Saint Petersburg, Russia; gemma.delafior@kit.edu

External Resource:  Presentation



MS-98-288-006_b.pdf

MS-99: Non-covalent interactions in crystal engineering II

Location: **Club D**

Session Chair: **Giuseppe Resnati**

Session Chair: **Petra Bombicz**

Invited: **Andrea Pizzi** (Italy), **Christian Jelsch** (France)

Introduction

2:45pm - 2:50pm

Introduction to session

Giuseppe Resnati, Petra Bombicz



MS-99-1833-001.pdf

2:50pm - 3:20pm

Seleninic acids as chalcogen bond donors: a molecular insight of GPx activity

Andrea Pizzi¹, Tripathi Abhishek^{2,3,4}, Andrea Daolio¹, Zhifang Guo³, David Turner^{3,4}, Glen Deacon^{3,4}, Harkesh Singh^{2,4}, Giuseppe Resnati¹

¹Politecnico di Milano, Milano, Italy; ²Indian Institute of Technology; ³Monash University; ⁴IITB-Monash Research Academy; andrea.pizzi@polimi.it

External Resource:  Presentation



MS-99-753-002_b.pdf

3:20pm - 3:50pm

Deciphering the driving forces in crystal packings by analysis of hydrogen bonds, electrostatic energies and contact enrichment ratios.

Christian Jelsch¹, Yvon Bibila Bisseyou², Benoît Guillot¹

¹CRM2 CNRS Université de Lorraine, Vandoeuvre les Nancy, France; ²University Felix Houphouet-Boigny, Abidjan, Côte d'Ivoire; christian.jelsch@univ-lorraine.fr

External Resource:  Presentation



MS-99-853-003_b.pdf

3:50pm - 4:10pm

The role of S-bond in tenoxicam keto-enolic tautomerization.

Sergey G. Arkhipov^{1,2}, Peter S. Sherin^{1,3}, Alexey S. Kiryutin^{1,3}, Vladimir A. Lazarenko⁴, Christian Tantardini⁵

¹Novosibirsk State University, Novosibirsk, Russian Federation; ²Boreskov Institute of Catalysis SB RAS; ³International Tomography Center; ⁴National Research Center "Kurchatov Institute"; ⁵Center for Energy Science and Technology, Skoltech Skolkovo Institute of Science and Technology; arksergey@gmail.com

External Resource:  Presentation



MS-99-296-004_b.pdf

4:10pm - 4:30pm

Evolution of halogen bonding interactions in a co-crystal system: X-ray diffraction under pressure in lab

Vishnu Vijayakumar-Syamala¹, Maxime Deutsch¹, Emmanuel Aubert¹, Massimo Nespola¹, Cyril Palin¹, Emmanuel Wenger¹, Arun Dhaka², Marc Fourmigue², Enrique Espinosa¹

¹Université de Lorraine, CNRS, CRM2, UMR 7036, Nancy 54000, France; ²Institut des Sciences Chimiques de Rennes (ISCR), UMR CNRS 6226, Université de Rennes 1, Campus de Beaulieu, 35042 Rennes, France; vishnu.vijayakumar-syamala@univ-lorraine.fr

External Resource:  Presentation



MS-99-278-005_b.pdf

4:30pm - 4:50pm

Tuning mechanical responses of crystalline cadmium(II) coordination polymers through cyano functionality and halide anions

Mateja Pisačić, Marijana Đaković

Faculty of Science, University of Zagreb, Zagreb, Croatia; mateja.pisacic@chem.pmf.hr

External Resource:



MS-99-475-006_b.pdf

4:50pm - 5:10pm

Halogen Bonding for Aromatic Hydrocarbon Assembly in the Solid State

Jogirdas Vainauskas, Tristan H. Borchers, Filip Topić, Tomislav Friščić

McGill University, Montreal, Canada; jogirdas.vainauskas@mail.mcgill.ca

External Resource:



MS-99-1157-007_b.pdf

5:10pm - 6:10pm

Afternoon break 7: Coffee/tea

Location: **Exhibition and poster area**

Poster - 48 Fragment screening: Fragment screening

Session Chair: **Alice Douangamath**

Session Chair: **Lisa J. Keefe**

5:10pm - 6:10pm

Poster session abstracts

Radomír Kužel



Poster - 48 Fragment screening-1975-001.pdf

Hundreds of starting points for spliceosomal PPI modulators identified by crystallographic fragment screening with the F2X-Universal Library

Tatjana Barthel^{1,3}, Jan Wollenhaupt¹, Gustavo M. A. Lima², Markus C. Wahl³, Manfred S. Weiss¹

¹Helmholtz-Zentrum Berlin, Macromolecular Crystallography, Albert-Einstein-Str. 15, 12489 Berlin, Germany; ²MAX IV Laboratory, BioMAX, Fotongatan 2, 224 84 Lund, Sweden; ³Freie Universität Berlin, Institute of Chemistry and Biochemistry, Laboratory of Structural Biochemistry, Takustraße 6, 14195 Berlin, Germany

External Resource:



Poster - 48 Fragment screening-1479-002_b.pdf

HIF-Prolyl-Hydroxylase 2 Clinical Inhibitor Complex Structure and XChem Fragment-Based Screen Obtained with Succinate Co-Product Used as a Crystallisation Tool.

William D. Figg Jr¹, Michael A. McDonough¹, Yu Nakashima^{1,3}, Rasheduzzaman Chowdhury^{1,2}, Christopher J. Schofield¹

¹Department of Chemistry, University of Oxford, Oxford, United Kingdom; ²Cardiovascular Research Institute, University of California, San Francisco, CA, United States; ³Institute of Natural Medicine, University of Toyama, Toyama, Japan

External Resource:



Poster - 48 Fragment screening-1404-003_b.pdf

Updates from FragMAX, a crystallographic fragment screening platform at MAX IV Laboratory

Tobias Krojer

MAX IV Laboratory, Lund University, PO Box 118, S-221 00 Lund, Sweden

External Resource:



Poster - 48 Fragment screening-1062-004_b.pdf

5:10pm - 6:10pm

Poster - 49 Non-covalent: Non-covalent interactions in crystal engineering

Session Chair: **Petra Bombicz**

Session Chair: **Giuseppe Resnati**

Poster session abstracts

Radomir Kužel



Poster - 49 Non-covalent-1976-001.pdf

How guest molecules affect on the self-assembly of carboxylated pillar[5]arene in its complexes

Helena Lidia Butkiewicz, Sandra Kosiorek, Volodymyr Sashuk, Oksana Danylyuk

Institute of Physical Chemistry Polish Academy of Sciences, Warsaw, Poland; hbutkiewicz@ichf.edu.pl

External Resource:



Poster - 49 Non-covalent-1401-002_b.pdf

Supramolecular arrangements in the crystal structures and the interaction energy calculations of resonance-assisted hydrogen-bridged (RAHB) rings - RAHB/RAHB and RAHB/C₆-aromatic contacts

Jelena Blagojevic Filipovic¹, Snezana Zaric²

¹Innovation Center of the Faculty of Chemistry, Belgrade, Serbia; ²Faculty of Chemistry, University of Belgrade, Serbia; jbfilipovic@chem.bg.ac.rs

External Resource:



Poster - 49 Non-covalent-449-003_b.pdf

Polymorphism and structural characterization of a Silver(I) coordination polymer: an inorganic-polymer co-former in the preparation of curcumin containing co-crystals

Francesca Scarpelli¹, Massimo La Deda¹, Giuseppe Di Maio¹, Renata De Rose¹, Iolinda Aiello¹, Mario Amati², Alessandra Crispini¹

¹Università della Calabria, Arcavacata di Rende, Italy; ²Università della Basilicata, Potenza, Italy; francesca.scarpelli@unical.it

External Resource:



Poster - 49 Non-covalent-862-004_b.pdf

A bug in enantiomer separation: double salt formation – diastereomeric and double salt structures of 1-cyclohexylethylammonium 2- and 4-chloromandelate

Sourav De¹, Laura Bereczki^{1,2}, Amit Zodge³, Márton Körösi³, Tamás Holczbauer^{1,4}, Edit Székely³, Petra Bombicz¹

¹Chemical Crystallography Research Laboratory, Research Centre for Natural Sciences, Hungary; ²Plasma Chemistry Research Group, Institute of Materials and Environmental Chemistry, Research Centre for Natural Sciences, Hungary; ³Department of Chemical and Environmental Process Engineering, Faculty of Chemical Technology and Biotechnology, Budapest University of Technology and Economics, Budapest, Hungary; ⁴Organocatalysis Research Group, Institute of Organic Chemistry, Research Centre for Natural Sciences, Hungarian Academy of Sciences, Budapest, Hungary; de.sourav@tkk.hu

External Resource:



Poster - 49 Non-covalent-1054-005_b.pdf

Structural study of Clopamide drug and copper (II) complexes under different crystallization conditions

G. Tamás Gál, Nóra V. May, Petra Bombicz

Centre for Structural Science, Research Centre for Natural Sciences, Budapest, Hungary; may.nora@tkk.hu

External Resource:



Poster - 49 Non-covalent-1211-006_b.pdf

Interaction between metallocene units

Goran A. Bogdanovic, Sladjana B. Novakovic

Vinca Institute of Nuclear Sciences, University of Belgrade, Belgrade, Serbia; goranb@vin.bg.ac.rs



Poster - 49 Non-covalent-118-007_b.pdf

Two sides of a molecular surface for analysis of non-covalent interactions

Anna V. Vologzhanina, Alexander A. Korlyukov

A.N. Nesmeyanov Institute of Organoelement Compounds, RAS, Moscow, Russian Federation; vologzhanina@mail.ru

External Resource:



Poster - 49 Non-covalent-1070-008_b.pdf

Synthesis and supramolecular analysis of novel purine alkaloid cocrystals with trimesic and hemimellitic acids

Mateusz Goldyn, Daria Larowska, Elżbieta Bartoszak-Adamska, Weronika Nowak

Department of Chemistry, Adam Mickiewicz University, 61-614 Poznań, Poland; mateusz.goldyn@amu.edu.pl

External Resource:



Poster - 49 Non-covalent-1696-009_b.pdf

Tailoring Crystal Structures and Polymorphs of Halogen-Bonded Supramolecular Assemblies: Co-Crystals of Hexahalogenated Benzenes and 2,3,5,6-Tetramethylpyrazine

Rama K. El-khawaldeh, Shubha S. Gunaga, David L. Bryce

Department of Chemistry & Biomolecular Sciences, University of Ottawa, Ottawa, Canada; relkh100@uottawa.ca

External Resource:



Poster - 49 Non-covalent-1421-011_b.pdf

Synthesis and single crystal structure determination of a new mixed-metal organic–inorganic hybrid of discrete transition metal halide complexes and α , ω -diammonioalkane assembled through non-covalent intermolecular interactions : $[\text{NH}_3(\text{CH}_2)_6\text{NH}_3]_4[\text{RhCl}_6][\text{FeCl}_4]\text{Cl}_4$

Mahsa Armaghan, Walter Frank

Heinrich Heine University of Duesseldorf, Düsseldorf, Germany; armaghan@uni-duesseldorf.de

External Resource:



Poster - 49 Non-covalent-1047-013_b.pdf

Influence of steric hindrance on the hydrates formation. The case of 2,2,6,6-tetramethylpiperidine and 3,3,5,5-tetramethylmorpholine

Paweł Socha, Bernadeta Prus, Łukasz Dobrzycki, Roland Boese, Michał Ksawery Cyrański

University of Warsaw, Warsaw, Poland; psocha@chem.uw.edu.pl

External Resource:



Poster - 49 Non-covalent-471-014_b.pdf

σ -hole interaction properties of divalent sulfur

Albert Singa Lundemba

University of Kinshasa, Kinshasa, Congo, Democratic Republic of the; albert.lundemba@unikin.ac.cd



Poster - 49 Non-covalent-393-015_b.pdf

Architecture of hydrogen-bonded anionic substructure vs cation type in thiazolium hypodiphosphates

Daria Barbara Budzikur, Katarzyna Anna Ślepokura

University of Wrocław, Wrocław, Poland; daria.budzikur@chem.uni.wroc.pl

External Resource:



Poster - 49 Non-covalent-1514-016_b.pdf

The crystal structure of four solvates of a bisphenol derivative.

Mizuki Fujino¹, Saori Gontani¹, Takeshi Nakamura², Shinya Matsumoto¹

¹Yokohama National University, Yokohama, Japan; ²Mitsubishi Chemical Corporation Osaka R&D Center, Osaka, Japan; fujino-mizuki-mr@ynu.jp

External Resource:





Poster - 49 Non-covalent-1474-017_b.pdf

Controlling π -Stacking Interactions in a Series of Novel Heteroacene Derivatives

Lana Klara Hiscock, Maly Kenneth, Dawe Louise
Wilfrid Laurier University, Waterloo, Canada; hisc2250@mylaurier.ca

External Resource: Presentation



Poster - 49 Non-covalent-1644-018_b.pdf

The first supramolecular consideration on crystal of DFMO – promising antiviral and anticancer pan-drug

Joanna Bojarska
Technical University of Lodz, Poland, Lodz, Poland; joanna.bojarska@p.lodz.pl



Poster - 49 Non-covalent-1884-019_b.pdf

Poster - 50 High Pressure: High Pressure Crystallography

Session Chair: **Przemysław Dera**
Session Chair: **Jon Henry Eggert**
Session Chair: **Lars Ehm**
Session Chair: **Vitali Prakapenka**



5:10pm - 6:10pm

Poster session abstracts

Radomír Kužel



Poster - 50 High Pressure-1977-001.pdf

EIGER2 CdTe detectors for hard X-ray research under extreme conditions

Tilman Donath, Max Burian, Stefan Brandstetter
DECTRIS Ltd., 5405 Baden-Daettwil, Switzerland; tilman.donath@dectris.com

External Resource: Presentation



Poster - 50 High Pressure-659-002_b.pdf

Completeness of data in XRD experiments using Diamond Anvil Cell

Daniel Tchou, Anna Makal
Faculty of Chemistry, University of Warsaw, Pasteura 1, 02-093 Warsaw, Poland; dtchou@chem.uw.edu.pl

External Resource: Presentation



Poster - 50 High Pressure-381-003_b.pdf

Pressure dependence of crystal and molecular structure and NLO response of L-Arg homologue salts.

Piotr Rejnhardt¹, Jan K. Zaręba², Andrzej Katrusiak³, Marek Daszkiewicz¹
¹Institute of Low Temperature and Structure Research, Polish Academy of Sciences, 50-950 Wrocław 2, P.O. Box 1410, Poland;
²Advanced Materials Engineering and Modelling Group, Faculty of Chemistry, Wrocław University of Science and Technology, Wybrzeże Wyspiańskiego 27, 50-370 Wrocław, Poland; ³Faculty of Chemistry, Adam Mickiewicz University, Umultowska 89b, Poznań, 61-614, Poland; p.rejnhardt@intibs.pl

External Resource: Presentation



Poster - 50 High Pressure-273-004_b.pdf

Reinvestigation of site-disorder in dense ice by *in-situ* neutron diffraction techniques

Keishiro Yamashita¹, Kazuki Komatsu¹, Stefan Klotz², Oscar Fabelo³, Maria Teresa Fernández-Díaz³, Jun Abe⁴, Shinichi Machida⁴, Tetsuo Irifune⁵, Takanori Hattori⁵, Toru Shinmei⁶, Kazumasa Sugiyama⁷, Toru Kawamata⁷, Hiroyuki Kagi¹
¹Geochemical Research Center, Graduate School of Science, The University of Tokyo, Hongo 7-3-1, Bunkyo-ku, Tokyo, 113-0033, Japan; ²IMPMC, UMR 7590, Sorbonne Université, Paris, France; ³Institut Laue-Langevin, Grenoble, France; ⁴Neutron Science and Technology Center, Comprehensive Research Organization for Science and Society, IQBRC Bldg, 162-1 Shirakata, Tokai, Naka, Ibaraki 319-1106, Japan; ⁵J-PARC Center, Japan Atomic Energy Agency, 2-4 Shirakata, Tokai-mura, Ibaraki 319-1195, Japan; ⁶Geodynamics Research Center, Ehime University, Matsuyama 790-8577, Japan; ⁷Institute for Materials Research, Tohoku University, Sendai, Japan; k1c.yamas@eqchem.s.u-tokyo.ac.jp

External Resource:



Poster - 50 High Pressure-1520-005_b.pdf

Uniaxial pressure in a High-resolution X-ray Diffraction environment

Vinicius E. S. Frehse^{1,2}, **Gustavo A. Lombardi**^{1,2}, **José C. Corsaletti Filho**¹, **Cris Adriano**², **Ricardo D. dos Reis**¹, **Guilherme A. Calligaris**¹

¹Brazilian Synchrotron Light Laboratory, Brazilian Center for Research in Energy and Materials, Campinas, SP, 13083-970, Brazil;

²Institute of Physics "Gleb Wataghin", University of Campinas – UNICAMP, 13083-859, Campinas, SP, Brazil; vinicius.frehse@lnls.br

External Resource:



Poster - 50 High Pressure-1509-006_b.pdf

In situ XRPD of the synthesis of corundum from boehmite during ball milling.

Tobias Rathmann¹, **Hilke Petersen**¹, **Steffen Reichle**¹, **Martin Etter**², **Amol P. Amrute**¹, **Wolfgang Schmidt**¹, **Claudia Weidenthaler**¹

¹Max-Planck-Institut für Kohlenforschung, Heterogeneous Catalysis, Kaiser-Wilhelm-Platz 1, 45470 Mülheim an der Ruhr, Germany;

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Poster - 50 High Pressure-1489-007_b.pdf

Polyamorphization-induced superconductivity in Sb₂Se₃

Wenge Yang

Center for High Pressure Science and Technology Advanced Research (HPSTAR), Shanghai, China, People's Republic of;
yangwg@hpstar.ac.cn

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Poster - 50 High Pressure-1709-008_b.pdf

New materials development utilizing mechanochemical synthesis

Phuong Quang Hoang Nguyen¹, **Warren McKenzie**¹, **Dongzhou Zhang**^{1,2}, **Jingui Xu**^{1,2}, **Robert Rapp**¹, **John Phillip Bradley**¹, **Przemyslaw Dera**¹

¹Hawaii Institute of Geophysics and Planetology, University of Hawaii at Manoa, Honolulu, Hawaii 96822, USA; ²GeoSoiEnviro CARS, Argonne National Laboratory, University of Chicago, Argonne, Illinois 60439, USA; nguyenph@hawaii.edu

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Poster - 50 High Pressure-1783-009_b.pdf



Poster - 50 High Pressure-1783-009_c.pdf

Exploring the high pressure bcc alloy phase of topological Insulator PbBi₄Te₇: synchrotron x-ray diffraction measurement and DFT simulations

Brahmanad Chakraborty^{1,2}, **Sumita Sura**², **Nandini Garg**^{1,2}

¹Bhabha Atomic Research Centre India, Mumbai, India; ²Homi Bhabha national institute Mumbai India; sumitasura.05@gmail.com

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Poster - 50 High Pressure-1706-010_b.pdf

Researches on pressure induced phase transitions using multiple synchrotron X-ray techniques: From crystalline to non-crystalline samples

Luhong Wang¹, **Arthur Haozhe Liu**²

¹Harbin Institute of Technology, Harbin, China, People's Republic of; ²HPSTAR, Beijing, China, People's Republic of;
haozhe@hit.edu.cn



Poster - 50 High Pressure-1656-011_b.pdf

5:10pm - 6:10pm

Poster - 51 Stimuli: Stimuli-responsive crystalline compounds



Session Chair: Chiara Massera
Session Chair: Ivan Halasz

Poster session abstracts

Radomír Kužel



Poster - 51 Stimuli-1978-001.pdf

Polymorphic tuning of a flexible organic crystal optical waveguide

Torvid Feiler^{1,2}, Biswajit Bhattacharya¹, Adam Michalchuk¹, Seon-Young Rhim², Vincent Schröder^{2,3}, Emil List-Kratochvíl^{2,3}, Franziska Emmerling^{1,2}

¹Federal Institute for Materials Research and Testing (BAM); ²Humboldt-Universität zu Berlin; ³Helmholtz-Zentrum Berlin für Materialien und Energie; Torvid.Feiler@bam.de

External Resource: Presentation



Poster - 51 Stimuli-1720-002_b.pdf

Mechanical Flexibility in 1D Coordination Polymer Crystals

Biswajit Bhattacharya, Adam Michalchuk, Franziska Emmerling

Bundesanstalt für Materialforschung und -prüfung (BAM), Berlin, Germany; biswajit.bhattacharya@bam.de

External Resource: Presentation



Poster - 51 Stimuli-1701-003_b.pdf

Mechanical-Bending-Induced Fluorescence Enhancement in Plastically Flexible Crystals of a GFP Chromophore Analogue

Saikat Mondal, C. Malla Reddy, Prasun K Mandal

IISER Kolkata, Mohanpur, India; mondalsaikat334@gmail.com

External Resource: Presentation



Poster - 51 Stimuli-710-004_b.pdf

Metal-like Ductility and Malleability in Organic Plastic Crystals

Amit Mondal, Biswajit Bhattacharya, Susobhan Das, Surojit Bhunia, Rituparno Chowdhury, Somnath Dey, C. Malla Reddy

IISER Kolkata, Mohanpur, India; amit.chem.mondal@gmail.com

External Resource: Presentation



Poster - 51 Stimuli-712-005_b.pdf

Poster - 52 Time-resolved: Time resolved phase evolution, interaction and crystallization in soft matter



5:10pm - 6:10pm

Session Chair: Jrjeng Ruan
Session Chair: Mitsuhiro Shibayama

Poster session abstracts

Radomír Kužel



Poster - 52 Time-resolved-1979-001.pdf

The organization of stable pre-crystallization phase from oligomers in lysozyme solution with different precipitates and the thin films formation at the air-liquid/air-substrate interfaces from the crystallization solutions

Margarita Marchenkova¹, Kseniia Ilina¹, Anastasiia Boikova¹, Petr Konarev¹, Alexey Seregin², Yulia Dyakova², Yury Pisarevskiy¹, Mikhail Kovalchuk²

¹Shubnikov Institute of Crystallography of Federal Scientific Research Centre "Crystallography and Photonics" of Russian Academy of Sciences; ²National Research Centre "Kurchatov Institute"; margaritkaepf@gmail.com

External Resource: Presentation



Poster - 52 Time-resolved-452-002_b.pdf

The formation of pre-crystallization oligomers in protein solutions during crystal growth

Kseniia Iliina¹, Anastasiia Boikova¹, Margarita Marchenkova¹, Yuri Pisarevskiy¹, Yulia Dyakova², Mikhail Kovalchuk²

¹Shubnikov Institute of Crystallography of Federal Scientific Research Centre "Crystallography and Photonics" of Russian Academy of Sciences; ²National Research Centre "Kurchatov Institute"; ilina-ks@mail.ru



Poster - 52 Time-resolved-454-003_b.pdf



Poster - 52 Time-resolved-454-003_c.pdf

Study of the behaviour of lysozyme oligomers in solutions by the molecular dynamics method at different temperatures

Iuliia Vladimirovna Kordonskaia^{1,2}, Vladimir Igorevich Timofeev^{1,2}, Yulia Alekseevna Dyakova^{1,2}, Margarita Aleksandrovna Marchenkova^{1,2}, Yura Vladimirovich Pisarevskiy^{1,2}, Mikhail Valentinovich Kovalchuk^{1,2}

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External Resource:



Poster - 52 Time-resolved-437-004_b.pdf

Evolution of heterogeneity and gelation of poly(*N*-isopropylacrylamide) aqueous solution at a temperature below cloud point

Atsuomi Shundo¹, Takuro Kogo², Chi Wang³, Keiji Tanaka^{1,2}

¹Department of Automotive Science, Kyushu University, Fukuoka, Japan; ²Department of Applied Chemistry, Kyushu University, Fukuoka, Japan; ³Department of Chemical Engineering, National Cheng Kung University, Tainan, Taiwan; a-shundo@cstf.kyushu-u.ac.jp

External Resource:



Poster - 52 Time-resolved-1246-005_b.pdf

Study on the intercalation of fullerene derivate into ordered phases liquid crystalline polymer

Chen-An Wang^{1,2}, Jrjeng Ruan², U-Ser Jeng^{1,3}

¹National Synchrotron Radiation Research Center (NSRRC), Hsinchu City, Taiwan; ²Department of Materials Science and Engineering, National Cheng Kung University, Tainan City, Taiwan; ³Department of Chemical Engineering, National Tsing Hua University, Hsinchu City, Taiwan; wang.ca@nsrrc.org.tw

External Resource:



Poster - 52 Time-resolved-1280-006_b.pdf

Poster - 53 Phase transitions: Structure and phase transitions in advanced materials

Session Chair: **Alexandra Gibbs**

Session Chair: **Yuichi Shimakawa**



5:10pm - 6:10pm

Poster session abstracts

Radomír Kužel



Poster - 53 Phase transitions-1980-001.pdf

Substitutional doping of trirutile transition metal antimonates, MSb₂O₆

Sneh Patel^{1,2}, Hyung-Been Kang¹, Helen Maynard-Casely³, Tilo Söhnel^{1,2}

¹School of Chemical Sciences, University of Auckland, 23 Symonds Street, Auckland 1010, New Zealand; ²Macdiarmid Institute for Advanced Materials and Nanotechnology, Victoria University of Wellington, Wellington 6140, New Zealand; ³Australian Centre for Neutron Scattering, Australian Nuclear Science and Technology Organisation, New Illawarra Road, Lucas Heights, NSW 2234, Australia; sp796@aucklanduni.ac.nz

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Poster - 53 Phase transitions-383-002_b.pdf

Tuning Expansion and Phase Transition Behavior in the Scandium Tungstate Family

Cora Lind-Kovacs, La'Nese Lovings, Dominik Dietzel

The University of Toledo, Toledo, United States of America; cora.lind@utoledo.edu

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Poster - 53 Phase transitions-589-003_b.pdf

Phase transition in CePt_2Al_2

Petr Doležal¹, Elen Duverger-Nédellec², Zuzana Mičková¹, Petr Proschek¹, Ksenia Illková³, Stanislav Daniš¹, Kristína Bartha⁴, Pavel Javorský¹

¹Charles University, Faculty of Mathematics and Physics, Department of Condensed Matter Physics, Prague, Czech Republic; ²CNRS, University Bordeaux, ICMCB, Pessac, France; ³Czech Academy of Sciences, Institute of Plasma Physics, Prague, Czech Republic;

⁴Charles University, Faculty of Mathematics and Physics, Department of Physics of Materials, Prague, Czech Republic; petr284@seznam.cz

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Poster - 53 Phase transitions-1149-004_b.pdf

Short-range charge density wave order in $\text{La}_{1.88}\text{Sr}_{0.12}\text{CuO}_4$ under uniaxial pressure

Ruggero Frison¹, Julia Kuespert¹, Qisi Wang¹, Niels Christensen², Jaewon Choi³, Oleh Ivashko⁴, Martin von Zimmermann⁴, Tohru Kurosawa⁵, Naoki Momono⁶, Migaku Oda⁵, Johan Chang¹

¹Physik Institut, University of Zurich, Winterthurerstrasse 190, CH-8057 Zurich, Switzerland; ²Department of Physics, Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark; ³Diamond Light Source, Harwell Science & Innovation Campus Didcot Oxfordshire OX11 0DE, United Kingdom; ⁴Deutsches Elektronen-Synchrotron DESY, Notkestraße 85, 22607 Hamburg, Germany;

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Poster - 53 Phase transitions-1116-005_b.pdf

Atomic mechanisms for the formation of charge-density waves in 3-dimensional electronic crystals

Sander van Smaalen¹, Sitaram Ramakrishnan¹, Srinivasan Ramakrishnan²

¹Laboratory of Crystallography, University of Bayreuth, Bayreuth, Germany; ²Department of Condensed Matter Physics and Materials Science, Tata Institute of Fundamental Research, Mumbai, India; smash@uni-bayreuth.de



Poster - 53 Phase transitions-435-006_b.pdf

Revisiting phase transitions in Ca-modified lead titanate ceramics using synchrotron XRD

Larissa Galao^{1,2}, Ducieli Garcia³, Flavia Regina Estrada¹

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³Physics Department, Federal University of São Carlos, São Carlos, Brazil.; flavia.estrada@lnls.br

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Poster - 53 Phase transitions-937-007_b.pdf

Temperature and time-resolved XANES studies of novel valence tautomeric cobalt complex

Svetlana Olegovna Shapovalova¹, Alexander Alexandrovich Guda¹, Mikhail Pavlovich Bubnov², Vladimir Kuzmich Cherkasov², Yuriy Vladimirovich Rusalev¹, Victor Vasilevich Shapovalov¹, Alexander Vladimirovich Soldatov¹

¹The Smart Materials Research Institute, Southern Federal University, Rostov-on-Don, Russian Federation; ²G. A. Razuvaev Institute of Organometallic Chemistry, Russian Academy of Sciences, Nizhny Novgorod, Russian Federation; cherkasova.svetlana.o@gmail.com

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Poster - 53 Phase transitions-521-008_b.pdf

Structural peculiarities of bismuth-containing $\text{RFe}_3(\text{BO}_3)_4$ ($\text{R} = \text{Ho}, \text{Y}, \text{Sm}, \text{Nd}$)

Ekaterina S. Smirnova¹, Olga A. Alekseeva¹, Alexander P. Dudka¹, Igor A. Verin¹, Vladimir V. Artemov¹, Dmitry N. Khmelenin¹, Irina A. Gudim², Kirill V. Frolov¹, Igor S. Lyubutin¹

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Poster - 53 Phase transitions-256-009_b.pdf

Modeling of lattice thermal expansion close to phase transitions: a DEA model extension.

Thorsten M. Gesing, Lars Robben, M. Mangir Murshed

University of Bremen, Institute of Inorganic Chemistry and Crystallography, Leobener Strasse 7, D-28359 Bremen, Germany;
gesing@uni-bremen.de



Poster - 53 Phase transitions-1405-010_b.pdf

Preferences of Chirality and Polarity in Triglycine sulfate Crystals

Yukana Terasawa¹, Toshio Kikuta², Masaaki Ichiki³, Sota Sato⁴, Kazuhiko Ishikawa⁵, Toru Asahi^{6,7}

¹School of Advance Science and Engineering, Waseda University, Tokyo, Japan; ²Faculty of Engineering, University of Toyama, Toyama, Japan; ³Research Center for Ubiquitous MEMS and Micro Engineering, National Institute of Advanced Industrial Science and Technology (AIST), Ibaraki, Japan; ⁴Department of Applied Chemistry, School of Engineering, The University of Tokyo, Tokyo, Japan; ⁵Graduate School of Advance Science and Engineering, Waseda University, Tokyo, Japan; ⁶Faculty of Science and Engineering, Waseda University, Tokyo, Japan; ⁷Research Organization for Nano & Life Innovation, Waseda University, Tokyo, Japan;
tinkerbelle@akane.waseda.jp



Poster - 53 Phase transitions-1284-011_b.pdf

Crystallography of silicon element: stable and metastable crystalline forms

Alexandre Courac (Kurakevych)

IMPMC - Sorbonne University, Paris, France; alexandre.courac@sorbonne-universite.fr

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Poster - 53 Phase transitions-637-012_b.pdf

Crystal Structure of Protic Ionic Liquids and their hydrates

Michael P. Hassett¹, Helen Brand², Jack Binns¹, Andrew V. Martin¹, Tamar L. Greaves¹

¹School of Science, RMIT University, Melbourne, Victoria 3000, Australia; ²Australian Nuclear Science and Technology Organisation, Australian Synchrotron, Victoria, 3168, Australia; s3717891@student.rmit.edu.au

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Poster - 53 Phase transitions-1088-013_b.pdf

Negative linear, in-plane zero and phase-transition-induced negative volume expansion in cranswickite-type $\text{MgSO}_4 \cdot 4\text{D}_2\text{O}$

Johannes M. Meusbürger^{1,2,3}, Karen A. Hudson-Edwards¹, Chiu C. Tang², Eamonn Connolly², Rich A. Crane¹, A. Dominic Fortes³

¹Camborne School of Mines and Environment and Sustainability Institute, Tremough Campus, University of Exeter, Penryn TR10 9EZ, UK; ²Diamond Light Source, Harwell Science and Innovation Campus, Fermi Avenue, Didcot OX11 0DE, UK; ³ISIS Neutron and Muon Source, STFC Rutherford Appleton Laboratory, Harwell Science and Innovation Campus, Chilton, Didcot, Oxfordshire, OX11 0QX, UK;
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Poster - 53 Phase transitions-1442-014_b.pdf

Two stages in one spin crossover in $[\text{Fe}(\text{bbtr})_3](\text{CF}_3\text{SO}_3)_2$

Maria Książek¹, Marek Weselski², Joachim Kusz¹, Robert Bronisz²

¹Institute of Physics, University of Silesia, 75 Pułku Piechoty 1, 41 – 500 Chorzów, Poland; ²Faculty of Chemistry, University of Wrocław, F. Joliot – Curie 14, 50 – 383 Wrocław, Poland; maria.ksiazek@us.edu.pl

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Poster - 53 Phase transitions-1508-015_b.pdf

Nitrile orientation versus crystal lattice as a tool for tuning the spin crossover properties in the one-dimensional coordination polymers $[\text{Fe}(\text{ebtz})_2(\text{RCN})_2](\text{BF}_4)_2$ (RCN = nitrile)

Joachim Kusz¹, Maria Książek¹, Marcin Kaźmierczak², Aleksandra Tołoczko², Marek Weselski², Robert Bronisz²

¹Institute of Physics, University of Silesia, 75 Pułku Piechoty 1, 41 – 500 Chorzów, Poland; ²Faculty of Chemistry, University of Wrocław, F. Joliot – Curie 14, 50 – 383 Wrocław, Poland; joachim.kusz@us.edu.pl

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Poster - 53 Phase transitions-1510-016_b.pdf

Operando PXRD and PDF Investigations of Disordering in NaCrO₂-CrO₂

Christian L. Jakobsen, Bettina P. Andersen, Dorthe B. Ravnsbæk
University of Southern Denmark, Odense C, Denmark; chril@sdu.dk

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Poster - 53 Phase transitions-1488-017_b.pdf



Poster - 53 Phase transitions-1488-017_c.pdf

Electrochemically driven phase transitions in crystallographically challenged electrode materials for rechargeable batteries

Martin Aaskov Karlsen, Dorthe Bomholdt Ravnsbæk
University of Southern Denmark, Campusvej 55, 5230 Odense M, Denmark; maak@sdu.dk

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Poster - 53 Phase transitions-1461-018_b.pdf

Crystal Structures and Phase Transitions of the Methylammonium Tin Halide Perovskites

Yui Fujihisa¹, Miwako Takahashi¹, Masato Hagiwara², Shuki Torii³, Takashi Kamiyama³, Takashi Ohhara⁴, Yukio Noda⁵
¹Faculty of Pure and Applied Sciences, University of Tsukuba, Tsukuba, 305-8573, Japan; ²Materials Sciences Research Center, Japan Atomic Energy Agency, Tokai, Ibaraki, 319-1195, Japan; ³Institute of Materials Structure Science, High Energy Accelerator Research Organization, Tokai, Ibaraki, 319-0016, Japan; ⁴J-PARC Center, Japan Atomic Energy Agency, Tokai, Ibaraki 319-1195, Japan; ⁵Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Sendai 980-8577, Japan; s2120357@s.tsukuba.ac.jp

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Poster - 53 Phase transitions-1503-019_b.pdf

Synthesis, crystal structure and catalytic activity of a new organic-inorganic hybrid cobalt phosphite

Mohamed AKOUBAA¹, Najlaa HAMD², Rachid OUARSAL³, Souâd RAKIB⁴, Brahim EL BALI⁵, Mohammed LACHKAR⁶

¹Engineering Laboratory of Organometallic, Molecular Materials and Environment (LIMOME) University Sidi Mohamed Ben Abdellah,; ²Engineering Laboratory of Organometallic, Molecular Materials and Environment (LIMOME) University Sidi Mohamed Ben Abdellah,; ³Engineering Laboratory of Organometallic, Molecular Materials and Environment (LIMOME) University Sidi Mohamed Ben Abdellah,; ⁴Engineering Laboratory of Organometallic, Molecular Materials and Environment (LIMOME) University Sidi Mohamed Ben Abdellah,; ⁵Independent scientist, Oujda, Morocco; ORCID: 0000-0001-6926-6286.; ⁶Engineering Laboratory of Organometallic, Molecular Materials and Environment (LIMOME) University Sidi Mohamed Ben Abdellah,; mohamed.akoubaa@usmba.ac.ma

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Poster - 53 Phase transitions-1639-020_b.pdf

Crystallographic studies of the spin state transition of three Fe(II) metallogrids: thermal vs ultra-fast photoswitching

Jose de Jesus Velazquez Garcia¹, Krishnayan Basuroy¹, Darina Storozhuk¹, Joanne Wong², Serhiy Demeshko², Franc Meyer², Robert Henning³, Simone Techert^{1,4}

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External Resource:



Poster - 53 Phase transitions-1662-021_b.pdf

Phase Transformations in Ti-Nb-Zr-Ta-O Beta Titanium Alloys with High Oxygen and Reduced Nb and Ta Content

Dalibor Preisler¹, Josef Stráský¹, Petr Hrcuba¹, Tereza Košutová¹, Milan Dopita¹, Michaela Janovská², Michal Hájek¹, Miloš Janeček¹

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External Resource:



Poster - 53 Phase transitions-1845-022_b.pdf



Poster - 53 Phase transitions-1845-022_c.pdf

Crystallization and nucleation study of transition metal struvite and related compounds

Stephanos Karafilidis, Tomasz M. Stawski, Franziska Emmerling
BAM Berlin (Bundesanstalt für Materialforschung und -prüfung), Berlin, Germany; stephanos.karafilidis@bam.de

External Resource:  Presentation



Poster - 53 Phase transitions-1718-023_b.pdf

α phase lamellae orientation relationship in metastable β titanium alloys

Petr Harcuba¹, Jana Šmilauerová¹, Václav Holý²

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External Resource:  Presentation



Poster - 53 Phase transitions-1891-024_b.pdf



Poster - 53 Phase transitions-1891-024_c.pdf

5:10pm - 6:10pm

Poster - 54 Methods: Methods

Date and time of the session to be determined.



Poster session abstracts

Radomir Kužel



Poster - 54 Methods-1981-001.pdf

Advances in the Parameter Space Concept for Crystal Structure Determination – a maximum resolution study

Matthias Zschornak^{1,2}, Christian Wagner^{1,2}, Melanie Nentwich³, Dirk C. Meyer¹, Karl Fischer⁴

¹TU Bergakademie Freiberg, Institut für Experimentelle Physik, Leipziger Str. 23, D-09599 Freiberg, Germany; ²TU Chemnitz, Institut für Physik, Reichenhainer Str. 70, D-09126 Chemnitz, Germany; ³DESY Photon Science, Notkestr. 85, D-22607 Hamburg, Germany;

⁴Universität des Saarlandes, Experimentalphysik, Campus A5 1, D-66041 Saarbrücken, Germany; matthias.zschornak@physik.tu-freiberg.de

External Resource:  Presentation



Poster - 54 Methods-1504-002_b.pdf

High-pressure CO₂ for lipid-mediated cocrystallization of theophylline and nicotinamide

Yuna Tatsumi, Yingquan Hao, Yusuke Shimoyama

Tokyo Institute of Technology, Tokyo, Japan; yshimo@chemeng.titech.ac.jp

External Resource:  Presentation



Poster - 54 Methods-1494-003_b.pdf

GIDInd: an automated indexing software for grazing-incidence X-ray diffraction data

Manuel P. Kainz², Lukas Legenstein², Valentin Holzer², Sebastian Hofer², Martin Kaltenecker², Roland Resel², Josef Simbrunner¹

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External Resource:  Presentation



Poster - 54 Methods-1350-004_b.pdf

Towards real-time analysis of liquid jet alignment in SFX

Jaydeep Patel¹, Adam Round², Andrew Peele³, Adrian Mancuso², Brian Abbey¹

¹La Trobe University; ²European XFEL; ³Australian Synchrotron (ANSTO); J.Patel2@latrobe.edu.au

External Resource:  Presentation



Poster - 54 Methods-1457-005_b.pdf

An efficient method for indexing grazing-incidence X-ray diffraction data of epitaxially grown thin films

Josef Simbrunner¹, Benedikt Schrode², Jari Domke³, Torsten Fritz³, Roman Forker³, Roland Resel²

¹Graz Medical University, Graz, Austria; ²Graz Technical University, Graz, Austria; ³Friedrich Schiller University Jena, Jena, Germany; josef.simbrunner@medunigraz.at

External Resource:



Poster - 54 Methods-1353-006_b.pdf

Development of microspectrophotometer for the macromolecular crystallography beamline at the Photon Factory, Japan

Masahide Hikita¹, Yusuke Yamada¹, Naohiro Matsugaki¹, Masahiko Hiraki², Toshiya Senda¹

¹Structural Biology Research Center, High Energy Accelerator Research Organization; ²Mechanical Engineering Center, High Energy Accelerator Research Organization; masahide.hikita@kek.jp

External Resource:



Poster - 54 Methods-1556-007_b.pdf

Growth of protein crystals in high-strength hydrogels with the dialysis membrane

Taichi Naruse¹, Kenta Hamada¹, Hiroaki Adachi², Tsugio Nagasawa³, Noriaki Kunimune³, Michio Murata⁴, Yusuke Mori⁵, **Shigeru Sugiyama¹**

¹Faculty of Science & Technology, Kochi University, Kochi, Japan; ²SOSHO Inc., Osaka, Japan; ³Kunimune Corp., Osaka; ⁴Graduate School of Science, Osaka University, Osaka, Japan; ⁵Graduate School of Engineering, Osaka University, Osaka, Japan; ssugiyama@kochi-u.ac.jp

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Poster - 54 Methods-1407-008_b.pdf

Development of Reciprocal Space Mapping Software for Single Crystal Diffraction

Yoshihisa Ishikawa¹, Ryoji Kiyonagi², Takashi Ohhara², Akiko Nakao¹, Koji Munakata¹, Kentaro Moriyama¹, Yukio Noda³

¹Comprehensive Research Organization for Science and Society, Tokai, Ibaraki, Japan; ²J-PARC center, Japan Atomic Energy Agency, Ibaraki, Japan; ³IMRAM Tohoku University, Sendai, Miyagi, Japan.; y_ishikawa@cross.or.jp

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Poster - 54 Methods-1601-009_b.pdf

Identifying problems in your single crystal diffraction data

Richard I. Cooper, David J. Watkin

University of Oxford, Oxford, United Kingdom; richard.cooper@chem.ox.ac.uk

External Resource:



Poster - 54 Methods-1694-010_b.pdf

Application of result of atoms and centrosymmetric cubic space groups for sharpening of Patterson function

Pui Sum Yuen

Nii, HONG KONG, Hong Kong S.A.R. (China); puiumyuen@netvigator.com

External Resource:



Poster - 54 Methods-1882-011_b.pdf

An attempt to find the use of atomic scattering factors and centrosymmetric cubic space groups; two choices of random phases in direct methods

Pui Sum Yuen

Nii, HONG KONG, Hong Kong S.A.R. (China); puiumyuen@netvigator.com

External Resource:



Poster - 54 Methods-1883-012_b.pdf

Poster - 55 XAFS: XAFS

Session Chair: **Paula Macarena Abdala**

Session Chair: **Marco Giorgetti**

5:10pm - 6:10pm



Poster session abstracts

Radomír Kužel



Poster - 55 XAFS-1982-001.pdf

Complex atomic fine structure in the phase domain: exciting opportunities and challenges

Chanh Quoc Tran¹, Christopher Thomas Chantler², Tony Kirk¹, Paul di Pasquale¹, Minh Hong Dao¹, Julian Ceddia¹, Zwi Barnea², Martin de Jonge³, Cameron Kewish³, David Paterson³

¹Department of Chemistry and Physics, La Trobe University, Bundoora, Victoria, Australia; ²School of Physics, University of Melbourne, Parkville, Victoria, Australia; ³XFM beamline, Australian Synchrotron, ANSTO, Clayton, Victoria, Australia; cq.tran@latrobe.edu.au

External Resource: Presentation



Poster - 55 XAFS-893-002_b.pdf

Dispersion Refinements in the Range of Absorption Edges

Florian Meurer¹, Florian Kleemiss¹, Oleg V. Dolomanov², Vedran Vukovic³, Horst Puschmann², Norbert Peyerimhoff⁴, Christoph Hennig⁵, Michael Bodensteiner¹

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External Resource: Presentation



Poster - 55 XAFS-1312-003_b.pdf

Solving Self-Absorption in Fluorescence

Ryan McEvey Trevorah, Christopher Thomas Chantler

University of Melbourne, Parkville, Australia; ryanmt@student.unimelb.edu.au

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Poster - 55 XAFS-425-004_b.pdf

X-ray absorption spectroscopy study of metal-organic frameworks functionalized by Pd: Formation and growth of Pd nanoparticles

Elizaveta Kozyr, Aram Bugaev, Alina Skorynina, Alexander Soldatov

Southern Federal University, Rostov-on-Don, Russian Federation; kamysnova.liza@gmail.com

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Poster - 55 XAFS-227-005_b.pdf

High accuracy determination of photoelectric crosssections, X-ray Absorption Fine Structure and nanostructure analysis of zinc selenide using the X-rayExtended Range Technique

Daniel Sier¹, Geoffrey P Cousland¹, Ryan M Trevorah¹, Ruwini S K Ekanayake¹, Chanh Q Tran², James R Hester³, Christopher T Chantler¹

¹University of Melbourne, Melbourne, Australia; ²La Trobe University; ³Australian Nuclear Science and Technology Organisation; dsier@student.unimelb.edu.au

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Poster - 55 XAFS-891-006_b.pdf

Facile synthesis of nano-structure LiCoPO₄@UiO-66 particles and its in-situ XAS, structural properties and electrochemical characterization for lithium batteries

Abdelaziz Aboraia, V. Shapovalov, A. Guda, V. Butova, A.V. Soldatov

Southern federal university, Rostov on-Don, Russian Federation; a.m.aboraia@gmail.com

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Poster - 55 XAFS-540-007_b.pdf

Mapping the thermo-induced valence tautomerism in Cobalt dioxolane single crystals

Ludmila Leroy¹, Lucas Pimenta¹, Leonardo Calazans¹, Marcos Ribeiro², Frederico Lima³, Simone Alexandre¹, David Shultz⁴, Majed Chergui⁵, Carlos Pinheiro¹

¹Physics department, Universidade Federal de Minas Gerais, 31270-901 Belo Horizonte, MG - Brazil; ²Chemistry department, Universidade Federal do Espírito Santo, Espírito Santo, ES - Brazil; ³European XFEL, Holzkoppel 4, 22869 Schenefeld, Germany; ⁴Department of Chemistry, North Carolina State University, Raleigh, NC 27695-8204, USA; ⁵Laboratoire de Spectroscopie Ultrarapide, ISIC-FSB-BSP, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland; ludmilaleroy14@ufmg.br

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Poster - 55 XAFS-492-008_b.pdf

PL-3: The structural biology of pathogenic amyloid fibrils

Location: **Panorama**

David Eisenberg

Video

The Expanding Amyloid Family: Structure, Stability, Function, and Pathogenesis

David Eisenberg

UCLA, Los Angeles, United States of America; david@mbi.ucla.edu

External Resource:  Presentation



PL-3-1916-001_b.pdf

Closing ceremony: Poster prizes, closing

Location: **Panorama**

Videos:

IUCr president - IUCr vicepresident - New IUCr president - Next congress - IUCr25 summary - Closing - Closing 2 -

Date: Sunday, 22/Aug/2021

Train trip Pilsen: Plzeň

Session Chair: **David Havlíček**

Prague (8:13 CHANGE - Pilsen, excursion in brewery, lunch, Pilsen - Prague (departure 15:22)

Date: Wednesday, 25/Aug/2021

Workshop - Resolution matters: Resolution Matters:- Discover the pathway from a high resolution 2D scan to the best phase analysis (Panalytical)

Location: **virtual**

2:00pm - 6:00pm

Join us on 25th August 2pm with Alejandro Rodríguez Navarro

Register Here: www.malvernpanalytical.com/IUCr2021

Date: Wednesday, 01/Sept/2021

School - Computing: Crystallographic Computing School

Location: **virtual**

Session Chair: **Martin Lutz**

2:00pm - 8:00pm

Session Chair: **Claudia Millán**

The Computing School will cover aspects that are relevant to all fields of crystallographic computing. As the main topic we will focus on the determination and the use of eigenvectors and eigenvalues and their applications in the different fields of crystallography. Applications range from the well known principal component analysis and other...

School - ePDF: School on electron PDF (pair-distribution function)

Location: **virtual**

Session Chair: **Tatiana Gorelik**

2:00pm - 8:00pm

virtual meeting

Date: Thursday, 02/Sept/2021

School - Computing 2: Crystallographic Computing School

Location: **virtual**

Session Chair: **Martin Lutz**

2:00pm - 8:00pm

Session Chair: **Claudia Millán**

The Computing School will cover aspects that are relevant to all fields of crystallographic computing. As the main topic we will focus on the determination and the use of eigenvectors and eigenvalues and their applications in the different fields of crystallography. Applications range from the well known principal component analysis and other...

School - ePDF 2: School on electron PDF (pair-distribution function)

Session Chair: **Tatiana Gorelik**

2:00pm - 8:00pm

virtual meeting

Date: Friday, 03/Sept/2021

School - Computing 3: Crystallographic Computing School

Location: **virtual**

Session Chair: **Martin Lutz**

2:00pm - 8:00pm

Session Chair: **Claudia Millán**

The Computing School will cover aspects that are relevant to all fields of crystallographic computing. As the main topic we will focus on the determination and the use of eigenvectors and eigenvalues and their applications in the different fields of crystallography. Applications range from the well known principal component analysis and other...

