



Czech and Slovak Crystallographic Association (CSCA)

Activities 2015 2017

In the period 2015-2017 the CSCA organized several meetings, seminars and conferences

One-day seminars - Rozhovory

297. ROZHOVORY

Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University Praha, 6. 2. 2015

60 years of Faculty of Nuclear Sciences and Physical Engineering,

V. Múčka: Powder diffraction at the Department of nuclear chemistry, V. Čuba: Synthesis of nanopowders and X-ray diffraction, J. Bárta: Preparation and research of nanoparticles of synthetic garnets, T. Pavelková: Radiation preparation of oxidic nuclear fuels, L. Procházková: Photo-induced preparation of nanoscintillators on the basis of ZnO and structural analysis, V. Jary: Scintillators based on ternary sulphides, P. Beran: Nano" and "quasi" in neutron diffraction, P. Oberta: Diffractometer Rigaku.

Exkursions in labs of Department of Nuclear Chemistry

Organization: N. Ganeev, V. Čuba

298. ROZHOVORY

Institute of macromolecular chemistry CAS in Prague
6. 11. 2015

Crystallography and X-ray methods of study of materials

V. Janovec: Does the study of domain structures belong to crystallography?, M. Rieder: What global statistics of mineralogic system can tell about crystallochemistry of elements, D. Korytár: X-ray crystal optics, E. Čaplovič: Structure and properties of hard coatings on tools. Structure analysis in the Institute of materials MTF STU in Trnava, P. Čapková: Combination of XRD and molecular modeling at structure solution of structures with limited order, J. Hašek: Application of XRD for solution of problems of structural biology within the framework of the project BIOCEV, E. Dobročka: Use of linear scans for analysis of epitaxial films. M. Steinhart: SWAXS at high pressures, R. Kužel: Strongly oriented thin magnetic films

Organization: J. Hašek, R. Kužel

299. ROZHOVORY

Institute of Materials - Faculty of Materials and Technology, Slovak Technical University, 12. 2. 2016

E. Čaplovič: Opening, short information on research infrastructure, I. Černíčková: Application of diffraction methods for study of structure of quasicrystalline approximant? P. Priputen: Use of X-ray methods for analysis of phase Y-Al₁₃Co₄ with complicated microstructure, M. Kusý: Microstructure and phase composition of quenched and tempered steels after hard lathing, M. Čaplovičová: Study of nanostructures with high-resolution transmission electron microscopy, L. Bónová: Plasma technologies at ATRI and possibilities of their use: R. Riedlmajer: Possibilities of ion implantation in laboratory of ion technologies, J. Dobrovodský: Analysis of materials at ATRI with the aid of ion beams including channelling

Excursion in the labs of Institute of Materials

Organizace: E. Čaplovič

300. ROZHOVORY

Institute of macromolecular chemistry CAS in Prague
11. 5. 2016

Anniversary 300th Rozhovory 25 years of CSCA

R. Kužel, J. Hašek: 25 years of the CSCA, B. Kratochvíl: Polymorphism in nature, J. Fiala: Low-temperature relaxation and secondary structure of material, E. Smrček: Structure refinement from powder - a view closely before retirement, M. Kotrlý: XRD phase analysis and other X-ray techniques in forensic practise, P. Strunz: Material research in Laboratory of neutron physics, Institute of Nuclear Physics Řež and planned neutron diffractometer BEER @ESS Lund, M. Dušek: Structure analysis in Institute of Physics, CAS: old cockpit has a new canvas and energetic crew, J. Moncol, J. Kožíšek: Interesting structures from data obtained by a new diffractometer STOE STADIVARI, study of electronic structure from diffraction data, J. Dohnálek: Structural biology in research center BIOCEV, P. Řezáčová: Integrative structural biology in Laboratory of structural biology at the Institute of Molecular Genetics and Institute of Chemistry and Biochemistry, CAS, I. Kutá Smanová: Laboratory of structural chemistry at University of South Bohemia in České Budějovice, P. Šutta: X-ray and electron diffraction on thin films with distorted perovskite structure, O. Caha: X-ray diffraction for the study of ferroelectric and piezoelectric thin films, R. Kužel: X-ray structure analysis at Faculty of Mathematics and Physics, Charles University. Some applications for study of materials

Organization: R. Kužel, J. Hašek



301. ROZHOVORY

BIOCEV, Institute of Biotechnology, CAS, Vestec
26. 4. 2017

Seminar devoted to the methods of study of molecular systems in the framework of EU projects BIOCEV (Common center of Czech academy of Sciences and Charles University in Vestec) and ELI (Extreme Light Infrastructure)

Joel L Sussman: Proteopedia - a world-wide source of knowledge of structure and function of proteins, B. Schneider: Structural dynamics of biomolecular systems, a joint ELI - IBT project, B. Angelov, J. Andreason: Present state and future of the X-ray diffraction station at ELI Beamlines, J. Dohnálek: The Czech Infrastructure for Integrative Structural Biology (CIISB), J. Pavlíček: Diffraction techniques in BIOCEV, J. Hašek: Software package provided by "Cambridge Crystallographic Data Centre", P. Pompach: Structural mass spectrometry (XR FT-ICR, MALDI, HPCL), A. Benda: Imaging methods, Z. Lánský: Experimental measurements intermolecular interactions – "optical tweezers"

Excursion in selected laboratories BIOCEV

Organization: J. Hašek, B. Schneider

302. ROZHOVORY

Institute of molecular biology SAS, Bratislava
11. 10. 2017

Protein crystallography, nothing more simple?

P. Pachl: Rutinosidase: journey toward the X-ray structure, M. Kugler: Structure-based design of human carbonic anhydrase inhibitors, J. Bauer: The structure and dynamics of the human ryanodine receptor 2 N-terminal domain and its mutants, D. Čierna: Characterization of domains of hu-

man ryanodine receptor 2 - better understanding of heart arytmiés, J. Škerlová: Crystal structure of native β -N-acetylhexosaminidase from *Aspergillus oryzae*: substrate specificity, stability, and regulation by propeptide, M. Nováková: Towards the structure of metabolic repressor DeoR from *Bacillus subtilis*, R. Škrabana: What can it look like to bind a glycine-rich epitope? O. Cehlár: Crystallographic insights into the binding of intrinsically disordered proline rich tau peptide to antibody Fab fragment, L. Urbániková: Atomic resolution and protein flexibility

Organization: E. Urbániková

Struktura 2015

Hotel Adamantino, Luhačovice

22. - 25. 6. 2015

Main lectures

M. Dušek: System for sample administration via Internet: a way from simple table to monster, J Brynda: High-resolution protein structure refinement, "glory and misery" of structure analysis of biomolecules, M. Babiak, J. Klumpler: Service of central laboratory of X-ray diffraction in CEITEC, Brno, BioSAXS CEITEC-MU in Brno, M. Kotrlý: Interesting cases on practice of Institute of Criminalistics, J. Drahokoupil: X-ray diffraction in practice, M. Jergel: Crystal optics for X-ray beam shaping, Z. Matěj: Integration of data from 2D detector at scanning powder diffraction experiment, J. Rohlíček: Structure solution from laboratory powder diffraction data - trends, possibilities, examples.

Structural databases

J. Hašek: 50 years of Cambridge structural database CSD, B. Schneider: 45 years of Protein structure databank PDB, J. Moncol: Use of CSD in Slovak universities F. Laufek:



Struktura 2015

Structure types and inorganic structure database, R. Kužel: Possibilities of use of new version of powder diffraction file - PDF-4+, open structure databases

Other Lectures, short contributions

M. Hříbová: The effect of some physical factors on the phase structure of isotactic polybutene -1, E. Dobročka: Measurement of residual stresses in strongly oriented thin films, M. Černík: X-ray diffraction analysis of coal and coke, J. Kopeček: Shape-memory alloys studied by EBSD, D. Šimek: Microstructure of drawn pearlitic steel and their image in XRD, M. Čerňanský: Laser working of materials, L. Horák: Study of (magneto-)structural transition in thin films FeRh studied by XRD, T. Roch: Structure characterization of heterostructures of metal oxide -based gas sensors, R. Uhrecký: The study of preparation of SrAl₁₂O₁₉ thin films, P. Vranec: XRD phase analysis of agglomerates, J. Novák: Variety and systematics of structures of binary mixtures of organic semiconductors, M. Meduňa: Reconstruction of shape of microcrystal with the aid of X-ray nanodiffraction on 3D multilayers, M. Šlouf: Application of Fourier transform for the analysis of microphotographs II, M. Dopita: X-ray scattering on strongly distorted carbon materials, J. Moncol: Self-ordering of copper carboxylates in supramolecular dimers and supramolecular networks with hydrogen bonds, E. Rakovský: Functionalization of polyoxometalates with complexes of transition metals, B. Schneider: Fine structure of DNA "duplex", E. Urbániková: Glucoamylases from *Saccharomycopsis fibuligera* - structure and stability, B. Vidová: Actinofage endolysins: bioinformatic analysis of domains and protein-substrate interactions, R. Chaloupková: Optimization of equilibrium between activity and stability of halogenalkane dehalogenases by engineering of their access tunnels, T. Prudnikova: Structural characterization of haloalkane dehalogenases

P. Oberta: New diffractometer Rigaku - SmartLab3, J. Gertenbach: News from Panalytical

P. Mikulík: European Synchrotron User Organisation (ESUO) and portal WayForLight.eu, R. Kužel: International year of crystallography and IUCr activities

11th student symposium from the field of crystallography and structure analysis

Biocrystallography and chemistry session

E. Škořepová: X-ray and NMR studies of protonated state of pharmaceutical amides, V. Sládková: Pharmaceutical cocrystals and their applications, I. Iermak: Structural characterization of glyceraldehyde dehydrogenase from *Thermo-plasma acidophilum*, D. Malakhova: Crystallization of novel haloalkane dehalogenase DgaA isolated from *Glaciicola agarilytica* NO₂, K. Tratsiak: Structural characterization of the representative of the alpha/beta-hydrolase superfamily from *Marinobacter* sp. ELB17, D. Jamrichová: Acetylsterases CE16 from *Hypocrea jecorina*

Awarded students: I. Iermak, D. Jamrichová, E. Škořepová

Materials and Physics session

M. Pšenička: Molecular simulations of interactions of nanoparticles CdS with montmorillonite, J. Rozbořil: X-ray diffraction study of stress relaxation in Ge microcrystals Ge, D. Kaščáková: Preparation and characterization of nanocomposites Fe₂O₃/SiO₂ substituted by Sc, M. Soroka: Preparation of oriented Co₃O₄ films by decomposition of Na₂CoO₂, J. Čapek: Determination of residual stress in duplex steel during thermomechanic working, M. Kučeráková: Study of texture of metagabro mylonite by neutron diffraction, M. Dudr: Comparison of structure of temperature and tension induced martensite in nitinol, P. Veřtát: XRD determination of coefficient of thermal expansion of scandated of rare earth compounds, J. Kašlík: High-temperature powder diffraction as a tool for monitoring of thermally-induced transformations -Fe₂O₃ in different atmosphere, P. Cejpek: Study of structure of Heusler alloys by X-ray methods, C. A. Correa: Accuracy of structure analysis of single nanocrystals by PEDT, T. Brunátová: Study of temperature stability of titanate nanotubes up to 800 °C, J. Šmilauerová: X-ray study of growth of omega phase particles in Ti alloys.

Awarded students: J. Rozbořil, C. A. Correa, J. Šmilauerová

Course - groups in crystallography I

R. Kužel, V. Petříček, E. Dobročka

Symmetry operations, groups, some properties, combinations of symmetry operations, multiplication tables. Point and space groups and their meaning, symmetry of 2D patterns (examples). Space groups, diagrams of symmetry elements, general position diagrams. Classes. Extinction rules, symmetry of diffraction patterns. Groups in higher dimensions, superspace, modulated structures. Symmetry of magnetic structures. Similarity of structures from the point of view of groups, Bärnighausen tree.

Abstracts:

<http://www.xray.cz/ms/bul2015-3.htm>

Number of participants: 82



Struktura 2016, Marian Čerňanský



Struktura 2016, Pavel Srb

Struktura 2016

Hotel Dvořák, Tábor

12. - 15. 9. 2016

25 years of the CSCA

History:

R. Kužel: 25 years of CSCA, F. Laufek: Crystallography before Laue

Main lectures

V. Petříček: Structure solution, J. Hašek: Dynamic theory of crystallization as a tool for control of architecture of protein crystals, L. Urbániková: Influence of mutations on structure and properties of proteins, J. Brynda: Carborane and metallacarborane inhibitors of Carbonic Anhydrase IX, promising compounds for therapy, Z. Matěj: Tools for study of nanomaterials by atomic pair distribution function, M. Kotrlý: Interesting examples of phase analysis in forensic practice, J. Kulda: Neutron scattering and its complementarity to X-ray diffraction, M. Hušák: Verification of determined structure of molecular crystals by QM-DFT calculations, P. Svoboda: Methods of inorganic crystal growth, I. Kutá Smatanová: How to prepare crystals of biological macromolecules? R. Kužel: Study of oriented films of hexagonal ferrites

Main lectures - related techniques

P. Srb: NMR and X-ray diffraction are not enemies any more, J. Čížek: Positron annihilation spectroscopy, A. Lančok: Non-traditional applications of Mössbauer spectroscopy, A. Macková: Energetic ion beams for characterization of composition and structure of crystalline materials for optics and photonics, V. Havránek: Ion microprobe - Analyses and modifications of materials by energetic beams, J. Čížek: 3D atom probe, P. Mikulík: X-ray imaging methods, S. Kamba: Use of infrared and Raman spectroscopy for refinement of crystal structures, M. Dopita: Method of electron-back scattered diffraction (EBSD), M. Černík: Texture and microstructure analysis by EBSD, J. Kopeček: Use of EBSD for study of shape-memory metals

Short contributions

P. Ryšánek: Structural characterization of polymer nanofiber textiles, I. Hren: Interaction of nylon 6 with antibacterial molecules, J. Drahekoupil: Nitridation of titanium by ion implantation, J. Maixner: Crystal structure of 3-amino-5-(aminocarbonyl)-2,4,6-triiodobenzoic acid methanol ($C_8H_5I_3N_2O_3 \cdot CH_3OH$) from laboratory powder data, T. Klumpler: Bio-SAXS - small-angle X-ray scattering on biological samples as a service of Central laboratories, M. Babiak: The crystallography of supramolecular complexes based on bambusuril, cucurbituril and similar macrocycles, J. Hybler: Some new findings on polytypism of mineral cronstedtit, M. Čerňanský: Approximation of Fourier coefficients of diffraction profiles, J. Čapek: Determination of residual stresses in duplex and austenitic steels, E. Samolová: Contribution to study of bimetallic compounds based on Mn(II) and Cu(II), A. Vráblová: Synthesis, characterization and crystal structure of two polymorph modifications $[Co_2(o-van-en)_3] \cdot 4CH_3CN$, P. Cejpek: Preparation and characterization of Ni_2MnGa doped with In, M. Pospíšil: Structures of Sr-phosphonated layers intercalated by alkanediols solved by methods of molecular simulations

Commercial contributions

R. Yellepedi (Thermo Scientific): Materials Analysis using Real-Time X-ray Diffraction and Advanced XRF, P. Oberta (Rigaku): Rigaku news, B. Míč (Měřicí technika Morava): Bruker X-ray products.

Number of participants: 55

Abstracts:

<http://www.xray.cz/ms/bul2016-4.htm>

Struktura 2017

Hotel Antoň, Telč

19. - 22. 6. 2017

Experimental methods in X-ray and neutron structure analysis

Lectures

R. Kužel: Introduction, notes to sources and detectors, R. Mokso: Imaging methods on synchrotrons and XFELs, J. Hybler: Single crystals methods with 2D registration, F. Laufek: Experience with position sensitive detector LynxEye XE, J. Moncol: Experience with diffractometer Stoe StadiVari with Ag and Cu microfocuse X-ray tubes for chemical crystallography, M. Dušek: Microfocus diffractometer in the Institute of Physics: experience, data evaluation in Jana 2006 and relations with detailed structure analysis, J. Rohlíček: Laboratory of powder diffraction in the Department of structure analysis of the Institute of Physics, CAS, E. Rakovský: Absence of knowledge of textbooks, P. Oberta: X-ray optics, D. Kriegner: Low-temperature diffractometry, L. Horák: X-ray characterization of epitaxial thin films, Z. Matěj: New nonstandard models in MSTRUCT and unconventional analysis, of nano-crystalline and amorphous like materials, P. Čápková: Re-



Struktura 2017

search service in the framework of research infrastructure NanoEnviCz, P. Ryšánek: Structure analysis on antibacterial filtration media, J. Novák: Growth and ordering of nanoparticles - as viewed by SAXS. Z. Zápražny: Diffraction surfaces of crystal monochromators prepared by nano-machining technique, E. Dobročka: Determination of threading dislocation density in epitaxial films of III-nitrides, P. Caha: X-ray diffraction on films of (Al,Ga)N ternary alloys, J. Kopeček: FeMnGa and NiMnGa alloys in the light of diffraction and microscopic techniques, T. Roch: Structural development of Ta-doped hard Ti-Al-N coatings, J. Drahokoupil: Ion implantation in titanium, M. Černík: New findings at solution of texture and structure by EBSD method, M. Čerňanský: Notes to evaluation of diffraction profiles, P. Beran: What's the matter between neutrons and matter?, D. Šimek: Statistical investigation of melting and growth of crystals, M. Kotrlý: Examples of phase microanalysis in forensic science, M. Jergel: Separation of phases polymer-fulleren by laboratory in-situ GISAXS and GIWAXS, J. Hašek: Dynamic theory of protein crystallization, J. Dohnálek: Development of protein diffractino technology, T. Skálová: NK cells, their receptors and interaction, J. Brynda, K. Pospíšilová: Second generation of inhibitors of carbon anhydrases on the basis of carboranes, P. Kolenko: Validation of ligands in macromolecular structures

Commercial contributions

B. Kinning (Xplorex): The Planet. Portable High-Resolution Powder Diffraction, D. Sisak Jung (Dectris): Technical specifications and your data: reading the lines and between the lines, P. Oberta (Rigaku): Rigaku 2017/18 news, A. Stricker (Incoatec): Upgrading Experimental Setups with Incoatec's Microfocus Source μ S and/or Scatterless Pinholes, A. Keilbach (Paar): Structure Analysis of Drug Delivery Systems with SAXS in the Laboratory, S. Prugovečki (Panalytical): Benchtop XRD PANalytical Aeris, J. Boutant (Xenocs): Latest developments in laboratory SAXS/WAXS instruments, T. Samtleben (Stoe): STOE – Tradition of Innovation since 1887, B. Mič (Měřicí technika Morava): Bruker X-ray products.



Struktura 2017, J. Hašek, L. Švecová

12th student symposium from the field of crystallography and structure analysis

Materials and Physics session

J. Čapek: Real structure of ferritic steels and ferritic phase in duplex steel after rolling, P. Veřtát: New phase close to i martensitic transformation in Ni-Mn-Ga, M. Dudr: XRD on high-entropy alloys, K. Trojan: Real structure and residual stresses in advanced welds determined by X-ray and neutron diffraction analysis, M. Čurda: Distortion of crystal structure of galenites by radioactive radiation ^{210}Pb , P. Cejpek: Preparation and study of structure of Ni_2MnGa alloys doped with In, J. Valenta: Low-temperature distortion of HoCo_2 , P. Doležal: Structural changes in intermetallic compounds $(\text{Ce,La})\text{Pd}_2(\text{Al,Ga})_2$, J. Rozbořil: In-situ X-ray diffraction annealing study on an anthradithiophene derivative

Awarded students: P. Veřtát, J. Rozbořil, P. Doležal



Biocrystallography session

K. Rejžková: Crystallization of protein Tt81 from *Thermococcus thio-reducens*, P. Havlíčková: Crystallization studies of protein Tt81 from *Thermococcus thio-reducens*, I. Berková: Crystallization studies of recently prepared haloalkane dehalogenase DgaA of *Glaciecola agarylitica* NO₂, L. Švecová: Bilirubin oxidase: Structural analysis of complexes with ligands in active place and study of activities, J. Stránský: A synchrotron tool used to process home source data, M. Malý: Diffraction limit in macromolecular crystallography, M. Hegedüs: Crystal structures of heterospin complexes based on Ni(II) and TCNQ, P. Masárová: Structural and spectroscopic study of copper(II) dipicolinate compounds, S. Matejová: Crystal structure of edaravone cocrystals

Awarded students: L. Švecová, M. Malý, M. Hegedüs

Number of participants: 87

Abstracts:

<http://www.xray.cz/ms/bul2017-1.htm>

CSCA was co-organizer of other meetings. This was for examples **Discussions in Structural Molecular Biology**, organized in Nové Hradý now also as annual meeting Czech Society for structural biology

www.structbio.org

XIII Discussions in Structural Molecular Biology

Academic and university centre Nové Hradý
19. 21. 3. 2015

Abstracts:

<http://www.xray.cz/setkani/abst2015/abstracts.htm> (html)

<http://www.xray.cz/ms/bul2015-1.htm> (pdf)

XIV Discussions in Structural Molecular Biology

Academic and university centre Nové Hradý
17. 19. 3. 2016

Abstracts:

<http://www.xray.cz/setkani/abst2016/abstracts.htm> (html)

<http://www.xray.cz/ms/bul2016-1.htm> (pdf)

The 1st FEBS-INSTRUCT Practical Crystallization Course in the Middle Europe entitled "Advanced Methods in Macromolecular Crystallization VI"

Academic and university center Nové Hradý, 20. 6.- 27. 6. 2014

The first FEBS-INSTRUCT Practical Crystallization Course held in the last week of June 2014 followed the first five successful FEBS courses of advanced crystallization courses held in 2004, 2006, 2008, 2010 and 2012. The course received an invitation from 24 leading world ex-

perts in protein crystallography, Prof. Bernhard Rupp of the Hofkristallamt of Vista (USA), Dr. Terese Berfors of Upsalla University (Sweden), Prof. Christian Betzel of the Univ.-Clinic Hamburg (Germany) and others. The event, organized under the auspices of FEBS (Federation of European Biochemical Societies) and INSTRUCT, sponsored 7 foreign and 1 Czech companies as well as the CSCA. In the morning lectures the students were acquainted with methods of isolation, purification and crystallization of proteins. During afternoon, in the framework of practical lessons, they tried everything they learned in lectures. Practical exercises were held at the site of the Laboratory of Biomolecular Crystalgenesis and Crystallography. During the one-week stay, besides the scientific program, there was also a cultural and social program, such as visiting the old castle in Nové Hradý. At the end of the course the students were evaluated his professional and social level in the form of a questionnaire and it can be stated that the participants were most satisfied with the course. The course, together with the Spanish Protein Crystallography School, was considered one of the best organized crystallization courses in the world. All information about the crystallization courses held in Nové Hradý is available at <http://febs.img.cas.cz>.

Abstracts were published in Materials Structure vol 21, no. 2a (2014), <http://www.xray.cz/ms/bul2014-2a.htm>

Number of student participants: 29

Number of lecturers: 26

Organizers:

Ivana Kutá Smatanová, Pavlína Řezáčová, Juan Manuel García-Ruiz.

"Advanced methods in macromolecular crystallization VII" - the 2nd FEBS practical crystallization course in the middle EU co-sponsored by INSTRUCT

Academic and University Center at Nove Hradý (Czech Republic)

June 27th to July 2nd, 2016

<http://febs.img.cas.cz>

The course was again organized under the main sponsorship of the FEBS and co-sponsored by INSTRUCT, however nine other companies sponsored the course mainly by contribution of material and providing their equipment for the lab exercises and also by paying of registration fee for four selected students (Czech Society for Structural Biology). Contributions of 32 lecturers/tutors with outstanding records in the field of protein crystallization and crystallography accepted organizer's invitation. Speakers together with organizers gave 28 morning lectures and 2 evening lectures. Students (24F and 15M) were welcomed by the dean of Faculty of Science of the University of South Bohemia as well as by the FEBS ACC chair and after this ceremony participants were introduced to standard and advanced methods of protein isolation and purification, nucleation, crystal morphology and growth mechanisms, crystallization screening and optimization using standard,



from FEBS course 2016

advanced and alternative crystallization techniques, seeding strategies, membrane protein crystallization, crystallization in microfluidic chips, crystal handling, mounting and cryocooling, fluorescent methods in crystallization, dynamic light scattering, neutron crystallography, approach to crystallizing proteins in the pharmaceutical industry as well as working with crystallization robot and measuring crystals using protein diffractometer. Lecture "Historical perspective on protein crystallization from 1840 to the present day", provided students by facts since past to now. During 4-hours afternoon practical exercises, focused on 15 different topics, students trained the freshly obtained knowledge and used standard and advanced crystallization methods to grow crystals of their own proteins (20 of them brought their own proteins) and/or selected model proteins. The course was absolutely successful for 2 students who were able to find initial crystallization conditions and grew crystals during the course. Participants were encouraged to present their projects during the course as a poster presentation. Twenty-nine posters were displayed during the whole duration of the course and poster session was organized as an evening event. The discussions during poster sessions have been very productive and helpful to all participants. Five posters were awarded by a poster prize – Bernhard Rupp's book given directly by Prof. Bernhard Rupp, two books by Prof. Juan Manuel García-Ruiz and other two books donated by the International Union of Crystallography. During the course Juan Manuel García-Ruiz has also supervised the exhibition CRISTALES installed directly on the caste foyer.

Majority of participants seemed to be very satisfied with scientific and social program of the course. Based on the positive responses from the feedback questionnaires, we are delighted to call the 2nd FEBS practical crystallization course in the middle EU co-sponsored by INSTRUMENT very

successful. We are looking forward to propose similar course scheduled for the year 2018.

Abstracts were published in Materials Structure vol 23, no. 2a (2016), <http://www.xray.cz/ms/bul2016-2a.htm>.

Number of student participants: 35

Number of lecturers: 32

Proteins in action - biophysical techniques for protein research

České Budějovice, Czech Republic, June 26-28, 2017

The Faculty of Science, USB, organized and hosted the first symposium on biophysical methods used for the study of proteins on 26-28 June. The main organizer was doc. Ivana Kutá Smatanová, with her organization assisted by dr. Pavlína Řezáčová (IOCB AS CR, Prague), dr. Jeroen Mesters (University of Lübeck, Germany) and prof. Beata Vertessy (Institute of Enzymology HAS Budapest, Hungary). The Symposium was called "Proteins in Action - Biophysical Techniques for Protein Research" and was designed to familiarize participants with the benefits of more rational approaches to use and a combination of different biophysical techniques to research the properties, function and structure of proteins. A number of prominent experts from various research disciplines have been invited. Our invitation was accepted by 11 lecturers from abroad and ten from the Czech Republic. In addition to the faculty, the symposium was also funded by XtalConcepts GmbH (Germany), NanoTemper Technologies Sp. z o.o. (Poland) and Eppendorf Czech & Slovakia s.r.o. from Czech republic. Representatives of the sponsoring companies lectured and



Proteins in Action

Pavína Malloy Řezáčová, Ivana Kutá Smatanová, Jeroen Mesters, Beata Vertessy

in the afternoon of the practical exercises they informed the participants about the use of their devices. Within the three-day symposium there were 26 lectures, two of them plenary and two students (selected from posters), and 4 laboratory exercises in which participants could test their own samples. The symposium was attended by a total of 65 participants, who eventually evaluated their level by means of a questionnaire. It can be said that everyone was very satisfied with the event so the organizers are considering another year that is likely to take place either in České Budějovice or Hamburg in 2019. All information about the symposium can be found at www.xray.cz/pa. Abstracts have been published in *Materials Structure*, vol.24, no. 2 (2017), <http://www.xray.cz/ms/bul2017-2.htm>.

Ivana Kutá Smatanová

Special group Solid state Chemistry and Physics

Development of Material Science i Research and Education

Main event organized is a seminar *Development of Materials Science in Research and Education (DMSRE)*. The first one took place in 1990 in Gabčíkovo. Since this year it is a regular meeting organized by the special group together with the Czechoslovak Association for Crystal Growth (CSACG) regularly moving between Czech and Slovak Republics, usually at the beginning of September. Other organizers are Faculty of Chemical and Food Technology STU Bratislava, Faculty of Materials and Technology in Trnava, CSCA, Regional committee of the Czech and Slovak Crystallographers and Slovak Society of Industrial Chemistry. In last years, just two places are changing - Pavlov in Czech Republic and Kežmarské Žlaby (Slovakia)

Programme is traditionally devoted to the following items:

- Trends in development of materials research.
- Education of materials science at the universities.
- Information about the research programmes of individual institutions.

- Information about equipment for preparation and characterisation of materials.

Participation is usually close to 40. Texts to the lectures are published in proceedings with the ISBN and/or in journal *CERAMICS - SILIKÁTY*.

Information on activities of the special groups can be found at <http://oschfil.bts.sk>. and about the conferences on the page of CSACG <http://csacg.fzu.cz/> resp. <https://dms.fzu.cz/>

Scientific Board of the CSCA

2017 2021

RNDr. Petr Bezdička, CSc. (1959)

Ústav anorganické chemie
Akademie věd České republiky, v.v.i., Praha

RNDr. Jiří Brynda, CSc. (1962)

Ústav molekulární genetiky
Akademie věd České republiky, v.v.i., Praha

RNDr. Milan Dopita, Ph.D. (1978)

Matematicko-fyzikální fakulta, Univerzita Karlova,
Praha

prof. Ing. Nikolaj Ganev, CSc. (1953)

Fakulta jaderná a inženýrská ČVUT, Praha

RNDr. Jindřich Hašek, DrSc. (1945)

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IUCr - International Union of Crystallography**IUCr commissions**

R. Kužel is a member of the IUCr executive committee since 2014. The following CSCA members are working in the IUCr commissions: Margarida Henriques (Institute of Physics CAS, Praha) - magnetic structures, Bohdan Schneider (Institute of Biotechnology CAS, BIOCEV Vestec) - biological macromolecules, Petr Bezdička (Institute of Inorganic Chemistry, Řež u Prahy), art and cultural heritage, Michal Dušek (Institute of Physics CAS, Praha) - aperiodic crystals, crystallographic nomenclature, International tables, Lukáš Palatinus (Institute of Physics CAS, Praha) – crystallographic computing and electron crystallography, Jozef Kožíšek (STU Bratislava) – quantum crystallography.

25th congress IUCr in Prague 2020

Congress will be held in August 22-30, 2020 in Prague Congress Centre.

Preparation of the congress has been started (www.iucr25.org or www.xray.cz/iucr). Main organizer is the CSCA, congress chair R. Kužel, chair of the International Programme Committee (IPC) is I. Kutá Smatanová, chair of the local organizing committee is P. Maloy Řezáčová and chair of the National Advisory Board is J. Hašek. There is collaboration with the PCO Aulettris (M. Haloun).

During spring 2018 the IPC should be defined. The IPC meeting should be held in spring 2019 in Prague and the conference programme should be prepared there. The IPC, selection of keynote lectures, topics of microsymbiosia and microsymbiosia chairs should be governed by the IUCr guidelines. The IPC composition is based on nominations by the IUCr commissions and should take into account geographical and gender balance.

International conferences organized by the CSCA**Aperiodic 2015****International Conference on Aperiodic Crystals**

*Břevnov Monastery, Prague, Czech Republic,
30 August – 4 September 2015*

The eighth of the triannual conferences Aperiodic devoted to all aspects of aperiodic crystals was held at fascinating spaces of the baroque Břevnov Monastery in Prague, Czech Republic. The conference was attended by 134 delegates from 25 different countries, 22 young scientists were supported from IUCr funding thank to the support of the Calendar Committee. Aperiodic 2015 was organized under the auspices of the Commission on Aperiodic Crystals of the International Union of Crystallography, the local organizer was the Czech and Slovak Crystallographic Association. Five days of the conference covered classical modulated structures, quasicrystals and magnetic struc-



Aperiodic 2015

tures, symmetry aspects, mathematical aspects, tiling theory, high pressure crystallography, diffuse scattering, lattice dynamics, physical properties, and commercial presentations. A special session was organized in memory of Chris Henley, one of the pioneers of the quasicrystal science who passed away recently. Honorary lecture “Usefulness and unusefulness of the superspace approach to aperiodic crystals” was held by the 2014 Ewald prize winner Ted Janssen, followed by an excursion to “Canada, two Americas and Mexico” or (alternatively) to the famous Křivoklát castle, both located in countryside close to Prague. Next Aperiodic will be organized in 2018 in Ames, Iowa, USA.

Conference web page <http://crysa.fzu.cz/aperiodic2015/>.

The abstracts of all lectures and poster presentations were published in *Materials Structure in Chemistry, Biology, Physics and Technology*, vol. 22, no. 4 (2015), <http://www.xray.cz/ms/bul2015-4.htm>.

ICCBM 16

International Conference on Crystallization of Biological Crystallization

*Hotel Pyramida, Prague, Czech Republic,
2–7 July 2016*

ICCBM conferences have been organized since 1985 in many countries all over the world. Prague was very proud for hosting the 16th International Conference on the Crystallization of Biological Macromolecules (ICCBM16) to bring experts from different fields interested in the crystallization of biological macromolecules. The topics of the conference aimed to cover all aspects of biological crystallogenesis from basic research on nucleation and crystal growth, to practical developments in crystallization methods and also advanced approaches.

The conference was organized by the International Organization for Biological Crystallization and the Czech and Slovak Crystallographic Association.

Participants of the ICCBM16 conference were welcomed by the dean of Faculty of Science of the University of South Bohemia as well as other organising bodies. After this cere-



ICCBM 16

Ivana Kutá Smatanová, Juan Manuel Garcia-Ruis, Pavlína Malloy Řezáčová, Jeroen Mesters



ICCBM 16

Terese Bergfors, Joe Ng

mony the program was followed by 14 different sessions focused on membrane protein crystallization, crystallization of macromolecular complexes, automation in crystallization, crystallization approaches for serial crystallography, chemistry of crystallization, complementary and scoring methods, teaching macromolecular crystallization, crystallization methods for neutron diffraction, theory and practice of crystallization and crystallization in industry and biomedicine. During the conference, Nobel Prize winner Prof. Ada Yonath from Weizmann Institute of Science



(Rehovot, Israel) accepted the invitation and gave lecture named The Recent Resolution Revolution & Friendly Medicine. This was organized as a public lecture and it was attended also by people who were not ICCBM16 participants. After the lecture, all could listen to the baroque music of Ars Instrumentalis Pragensis. Another public lecture named The impact of crystals in art and mind, was given by Prof. Juan Manuel García-Ruiz.

In addition to oral presentations, participants were encouraged to present their projects as a poster presentation. Seventy-two posters were displayed in two parts during the conference as an evening event. The discussions during poster sessions have been very productive and helpful to all participants. Five posters were awarded by a poster prize. During the course Prof. Juan Manuel García-Ruiz has also supervised the exhibition of 12 artistic posters introducing crystals to wide audience, CRISTALES, installed in the hotel foyer during the conference.

The abstracts of all lectures and poster presentations were published in a special issue of Bulletin of Czech and Slovak Crystallographic - MATERIALS STRUCTURE in Chemistry, Biology, Physics and Technology, vol. 23, no. 2 (2016), 111 pages (ISSN 1211 – 5894 (print), ISSN 1805 – 4382 (online)), <http://www.xray.cz/ms/bul2016-2.htm>.

According participant's references we are glad to say that participants spent illuminating week in Prague and enjoyed the science as well as some leisure time in Prague, a town with magnificent history and charm.

All information including conference photos can be found at the conference webpage:

Conference web page <http://www.xray.cz/iccbm/>
or <http://www.iccbm16.org>

Ivana Kuta Smatanova, conference chair

Pavlina Rezacova, conference co-chair

Radek Kuzel and Jindrich Hasek, CSCA representatives .

XTOP 2016

13th Biennial Conference on High-Resolution X-Ray Diffraction and Imaging

Cinema Scala, Brno, 4. – 8. 9. 2016

The XTOP conferences are organized every two years since 1992 by european research groups which are acknowledged by their work in the field of methods of x-ray scattering, X-ray imaging and instrumentation with both laboratory and synchrotron sources. The XTOP conference took place in the Czech Republic for the second time. This one in Brno has been organized by the Czech and Slovak Crystallography Association, Masaryk University (MU) and CEITEC MU. The conference place was the university cinema Scala, and thus participants could have enjoyed a large screen and great acoustics during lectures. Catering during breaks has been managed by the cinema bar, lunches and poster refreshment by the MU canteen, while two conference dinners took place in the Velká Klajdovka

hotel and the Pivovarská restaurace (Brewery restaurant) Starobrnno.

There were 150 delegates and 10 company sponsors. Local organizing committee has been supported by the international Scientific advisory board of 15 renowned scientists, defining the main topics and selecting the program and post-conference papers.

As in the previous XTOP conferences, we organized a one-day pre-conference school intended mainly for students and young researchers in order to present modern topics in more details which it is not possible during short conference talks. Selected topics about X-ray methods and instrumentation were presented in six talks of 80+20 minutes. These invited tutorials dealt with principles, experiments and applications of modern X-ray imaging methods, scanning methods with nanobeams, methods using phase contrast, energy-tunable sources, and advances in synchrotron sources and laboratory instrumentation.

Scientific program of the conference was distributed into 12 lecture and 2 evening poster sessions. Altogether there were presented 11 invited talks of 40 minutes, 42 short talks of 20 minutes, and 98 posters. Although the x-ray scattering and imaging methods are in development for more than 100 years, there are still many new features to discover and develop. As we cannot write about all of them in detail, let us mention at least some of them. Modern instrumentation leads to higher measurement speed necessary for in-situ and in-operando studies. Experiments exploiting high coherence of synchrotron beam leads to coherent imaging methods with phase and absorption contrast, which requires a sophisticated approach for reconstruction processes. Classical diffraction or small-angle scattering experiments were presented mainly in conduction with mapping of the reciprocal space of nanostructures or thin films using two-dimensional detectors. Further contributions dealt with structural studies of alloys or biological macromolecules, structures for semiconductor applications or systems for X-ray optics. Some of the contribution were theoretical as well.

Abstracts of all of the 147 accepted talks and posters were published in a special issue of Materials Structure, volume 23, number 3 (2016), <http://www.xray.cz/ms/bul2016-3.htm>.

Selected papers of conference participants were peer reviewed and published with an open access in the special issue in Journal of Applied Crystallography in June 2017, volume 50, see <http://journals.iucr.org/j/issues/2017/03/00/>.

More information as well as conference photos and videos can be found at the conference web page <http://xtop2016.sci.muni.cz/>.

Petr Mikulik, conference chair