Electron Crystallography School - 3D Electron Diffraction/MicroED Uniting Small Molecule and Macromolecular Crystallography

The real session on Aug. 14 is at the Prague Congress Center, the IUCr congress venue.

Organisers: Xiaodong Zou and Hongyi Xu, Sweden; Louisa Meshi, Israel; Lukas Palatinus, Czech Republic

School on 3D electron diffraction/MicroED techniques and how to apply them for structure determination of nano/microcrystals too small for X-ray diffraction. The topics will cover inorganic compounds, pharmaceutics and proteins. It includes both lectures and practical demonstrations. The following topics will be covered:

- The development of various 3D electron diffraction/MicroED techniques – a historical perspective
- Introduction to transmission electron microscopy and electron diffraction
- 3D electron diffraction/MicroED techniques and space group determination
- Sample preparation for both materials and life sciences
- 3D ED/MicroED Data collection including practical demo labs
- Radiation damage
- 3D ED Data Processing and data merging including practical demo labs
- Methods for phasing diffraction data – small molecules and macromolecules
- Practical demo labs for structure solution and refinement with 3D ED/MicroED data, for both small molecules and macromolecules
- Dynamical refinement
- New developments in 3D electron crystallography

<table>
<thead>
<tr>
<th>Chair</th>
<th>Xiaodong Zou</th>
</tr>
</thead>
<tbody>
<tr>
<td>09:00-09:30</td>
<td>Xiaodong Zou</td>
</tr>
<tr>
<td>09:30-10:00</td>
<td>Ute Kolb</td>
</tr>
<tr>
<td>10:00-10:30</td>
<td>Sven Hovmöller</td>
</tr>
<tr>
<td>10:30-10:45</td>
<td>Break</td>
</tr>
<tr>
<td>Chair</td>
<td>Ute Kolb</td>
</tr>
<tr>
<td>10:45-11:15</td>
<td>Enrico Mugnaioli</td>
</tr>
<tr>
<td>11:15-11:45</td>
<td>Jan Pieter Abrahams</td>
</tr>
<tr>
<td>11:45-12:15</td>
<td>Koji Yonekura</td>
</tr>
<tr>
<td>12:15-13:15</td>
<td>Lunch</td>
</tr>
<tr>
<td>Chair</td>
<td>Tom Willhammar</td>
</tr>
<tr>
<td>13:15-13:45</td>
<td>Joke Hadermann</td>
</tr>
<tr>
<td>13:45-14:15</td>
<td>Sven Hovmöller</td>
</tr>
<tr>
<td>14:15-14:45</td>
<td>Louisa Meshi</td>
</tr>
<tr>
<td>14:45-15:00</td>
<td>Break</td>
</tr>
<tr>
<td>Chair</td>
<td>Joke Hadermann</td>
</tr>
<tr>
<td>15:00-15:45</td>
<td>Hongyi Xu</td>
</tr>
<tr>
<td>15:45-16:15</td>
<td>Brent Nannenga</td>
</tr>
<tr>
<td>16:15-17:00</td>
<td>Tom Willhammar</td>
</tr>
<tr>
<td>17:00-17:15</td>
<td>Break</td>
</tr>
<tr>
<td>Chair</td>
<td>Hongyi Xu</td>
</tr>
<tr>
<td>17:15-17:45</td>
<td>Tamir Gonen</td>
</tr>
<tr>
<td>17:45-18:30</td>
<td>Sponsor session</td>
</tr>
</tbody>
</table>
### Thursday August 12

**Chair**
- Ronan Keegan

#### 9:00-9:45
- David Waterman
  - ED Data Processing theory

#### 9:45-10:30
- David Waterman
  - Dials – software demo

#### 10:30-10:45
- **Break**

**Chair**
- Lukas Palatinus

#### 10:45-11:30
- Kay Diederichs
  - XDS – software demo

#### 11:30-12:15
- Stef Smeets
  - Serial rotation electron diffraction: Automated high-throughput data collection and data processing

#### 12:15-13:15
- **Lunch + meeting companies in breakout rooms**

**Chair**
- Lukas Palatinus

#### 13:15-14:00
- Junliang Sun
  - Methods for phasing diffraction data – small molecules

#### 14:00-14:45
- Lukas Palatinus
  - Kinematical and dynamical structure refinement and absolute structure

#### 14:45-15:30
- Horst Puschmann
  - Olex2 for structure solution and refinement – software demo

#### 15:30-15:45
- **Break**

**Chair**
- Lukas Palatinus

#### 15:45-16:30
- Isabel Uson
  - Different methods for phasing diffraction data – macromolecules

#### 16:30-17:15
- Airlie McCoy
  - Phaser - molecular replacement - Theory

#### 17:15-18:00
- Ronan Keegan
  - CCP4 Phasing and Structure solution, Mr Bump

#### 18:00-18:30
- **Poster presentations**
  - 4 posters x 2 min/each, presentation order given in the end

### Friday August 13

**Chair**
- Hongyi Xu

#### 09:00-09:45
- Garib Murshudov
  - Refinement of macromolecular structures against electron diffraction data

#### 09:45-10:30
- Keitaro Yamashita
  - Coot – model building and refinement

#### 10:30-10:45
- **Break**

**Chair**
- David Watermann

#### 10:45-11:30
- Tristan Croll
  - ISOLDE – Interactive model building by molecular dynamics for low resolution data

#### 11:30-12:15
- Fraser White
  - Synergy-ED and CrysAlisPro: data collection, data processing and structure solution - demo

#### 12:15-13:15
- **Lunch + poster sessions**

**Chair**
- Louisa Meshi

#### 13:15-14:00
- Lukas Palatinus
  - PETS and Jana2006: Data processing and structure determination - software demo

#### 14:00-14:45
- Lukas Palatinus
  - Dynamical Refinement - software demo

#### 14:45-15:00
- **Break**

**Chair**
- Tristan Croll

#### 15:00-15:45
- Pavel Afonine
  - Phenix: refinement and validation

#### 15:45-16:30
- Pavel Afonine
  - Phenix – software demo

**Chair**
- Louisa Meshi

#### 16:30-17:00
- **Q & A**

---

### New developments and possibilities of electron crystallography (speakers on-site at the conference venue + virtual)

**Chair**
- Lukas Palatinus

#### 14:00-14:20
- Eric van Genderen
  - Detectors for crystallography, is there perfection?

#### 14:20-14:40
- Robert Bükker
  - Serial and scanning diffraction: chances and challenges

#### 14:40-15:00
- Richard Beanland
  - Prospects for improved quantitative electron diffraction

#### 15:00-15:20
- Paulina Dominiak
  - The potential hidden in the 3D ED data

#### 15:20-15:40
- Xiaodong Zou
  - 3D electron diffraction/MicroED: current status and future perspectives

#### 15:40-16:00
- **Coffee break**

#### 16:00-17:00
- Round table discussions – the future of 3D ED/MicroED

#### 17:00-17:15
- Poster award and concluding remarks

#### 17:30
- Opening of IUCr2021

*All speakers in this session are expected on-site in Prague. All school participants can attend either virtually or in person.*
Poster presentation order on August 12, 2 min/person:

1. Angotzi Marco Sanna
2. Bengtsson Viktor
3. Broadhurst Edward Thomas
4. Budniak Ursula
5. Cho Jungyoun
6. Ge Meng
7. Gruza Barbara
8. Kulik Marta
9. Kunal Kumar Jha
10. Li Yan
11. Pacoste Laura
12. Poppe Romy
13. Tirado Cañño Juan Ignacio
14. Vandemeulebroucke Daphne