



UNIVERSITÀ DI PISA



crystals

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ASSOCIAZIONE ITALIANA
CRISTALLOGRAFIA

3rd-6th July 2023
University of Pisa, IT



ELECTRON CRYSTALLOGRAPHY

a deep dive into nanocrystals

International School of Crystallography AICS2023

3rd July (day 1)

- 9:00 – 9:15 Welcome
Paolo P. Mazzeo, Mauro Gemmi
- 9:15 – 10:30 Crystallography and diffraction: Introduction to crystallography, a crystal in real and reciprocal space, the diffraction as a tool, with a direct reference always to electrons
Enrico Mugnaioli
- 10:30 – 11:00 Coffee break
- 11:00 – 11:45 The TEM as a diffractometer: Introduction to the TEM instrument, electron optics, imaging and diffraction, how a TEM works
Mauro Gemmi
- 11:45 – 12:30 Diffraction from accelerated electrons: geometry of electron diffraction, SAED, NED, precession electron diffraction and 3D ED as final goal
Enrico Mugnaioli
- 12:30 – 14:00 Lunch
- 14:00 – 15:30 3D ED data collection: different possible data collections type with ED
Mauro Gemmi
- 15:30 – 16:00 Coffee break
- 16:00 – 17:30 3D ED data reduction and analysis
Petr Brazda
- 18:00 Welcome party at
Bistrot Vettovaglie
Piazza S. Omobono, 22

4th July (day 2)

- 9:00 – 10:45 Structure solution with 3D ED data
Benedetta Carrozzini
- 10:45 – 11:00 Coffee break
- 11:00 – 12:30 Kinematical structural refinement with 3D ED data: how to refine a crystal structure kinematically
Tim Gruene
- 12:30 – 14:00 Lunch
- 14:00 – 17:30 Practical session
a Kinematical refinement with SHELX *Gruene, Faye, Marchetti*
b Structure solution with SIR *Carrozzini, Gemmi*
c Data analysis with PETS2 *Brazda, Faye, Marchetti*
- 15:30 – 16:00 Coffee Break

5th July (day 3)

- 9:00 – 9:45 Dynamical refinement
Petr Brazda
- 9:45 – 10:30 Structure analysis of inorganic compounds
Mauro Gemmi, Enrico Mugnaioli
- 10:30 – 11:00 Coffee break
- 11:00 – 11:45 Structure analysis of organic compounds
Tatiana Gorelik
- 11.45 – 12.30 Challenging problems and 3D ED data: small molecules, H determination, absolute structure
Petr Brazda
- 12:30 – 14:00 Lunch
- 14:00 – 14.30 3DED/MicroED made easy using the XtaLAB Synergy ED
James Gordon
- 14.30 – 18.00 Practical session
Group 1
a Data analysis with PETS2 *Brazda, Faye, Marchetti*
b Kinematical refinement with SHELX *Gruene, Faye, Marchetti*
c Structure solution with SIR *Carrozzini, Gemmi*
Group 2
a Instrument tour *Mugnaioli, Paoli, Alderighi*
b Dynamical refinement with JANA *Brazda, Gemmi*
- 16.00 – 16:30 Coffee Break
- 20:00 Social Dinner
OSTERIA I SANTI
Via Santa Maria 71/73

6th July (day 4)

- 9:00 – 10:30 3D ED for macromolecules
Gerhard Hofer
- 10:30 – 11:00 Coffee break
- 11:00 – 11:45 Texture and phase analysis: (ASTAR), 4D STEM
Muriel Veron
- 11.45 – 12.30 Disorder quantification and 2D crystals
Tatiana Gorelik
- 12:30 – 14:00 Lunch
- 14:00 – 16:00 Practical session
a Dynamical refinement with JANA *Brazda, Gemmi*
b Instrument tour *Mugnaioli, Paoli, Alderighi*
- 16:00 – 17:00 Final Round Table