

# Electron Crystallography - A deep dive into nanocrystals

*Pisa 3<sup>rd</sup>-6<sup>th</sup> July 2023*

## 3<sup>rd</sup> July (day 1)

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9:00 – 10:45 **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*

10:45 – 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 – 15:45 **3D ED data collection: different possible data collections type with ED**  
*Mauro Gemmi*

15:45 – 16:00 Coffee break

16:00 – 17:30 **3D ED data reduction and analysis**  
*Petr Brazda*

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## 4<sup>th</sup> July (day 2)

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9:00 – 10:45 **Structure solution with 3D ED data**

*Benedetta Carrozzini*

10:45 – 11:00 Coffee break

11:00 – 12:45 **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**

Group 1

**a Kinematical refinement with SHELX** *Gruene, Faye, Marchetti*

**b Structure solution with SIR** *Carrozzini, Gemmi*

**c Data analysis with PETS2** *Brazda, Faye, Marchetti*

Group 2

**a Structure solution with SIR** *Carrozzini, Gemmi*

**b Data analysis with PETS2** *Brazda, Faye, Marchetti*

**c Kinematical refinement with SHELX** *Gruene, Faye, Marchetti*

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## 5<sup>th</sup> July (day 3)

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9:00 – 9:45 **Dynamical refinement**

*Petr Brazda*

9:45 – 10:30 **Structure analysis of inorganic compounds**

*Mauro Gemmi, Enrico Mugnaioli*

10:45 – 11:00 Coffee break

10:45 – 11:30 **Structure analysis of organic compounds**

*Tatiana Gorelik*

11:30 – 12:15 **Challenging problems and 3D ED data: small molecules, H determination, absolute structure**

*Petr Brazda*

12:30 – 14:00 Lunch

14:00-17.30 **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

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## 6<sup>th</sup> July (day 4)

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**9:00 – 10:45 3D ED for macromolecules**

*Gerhard Hofer*

10:45 – 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 tou** *Mugnaioli, Paoli, Alderighi*

**16:00 – 17:00 Final round table**

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