

School Programme

Monday, 1st June

9:00 - Fernando J. Lahoz & Horst Puschmann (60 min)

Course Opening - 'Breaking the ice' - Motivational Stuff

10:00 - Fernando J. Lahoz (60 min)

Best Data for all Seasons... and Crystals

11:30 - Jakub Wojciechowski (120 min)

Obtaining the Best HKL Intensities when Crystals are not the Best Ones: Proper Data Collection, Reduction and Integration

15:30 - Duane Choquesillo (90 min)

Practical Crystallization Techniques and New Routes to Suitable Single Crystals

17:30 - Sergi Plana (90 min)

Alternative Radiations: The Case of ED ... including practical data treatment & refinement

19:00 - Fernando, Horst, Jakub & Sergi
Open Discussion Session

Tuesday, 2nd June

9:00 - Jakub Wojciechowski (120 min)

General Introduction to Twinning with some Practical Cases using CrysAlisPro

11:30 - Duane Choquesillo & Pilar García (120 min)

Practical session on Twinning using APEX

15:30 - Sergi Plana & Horst Puschmann (90 min)
Dealing ED Data: Dynamical Refinement with Olex2

17:30 - Horst Puschmann (90 min)

New tricks in Olex2 to Treat Problematic Data and Disorders

19:00 - Jakub, Duane, Sergi and Horst
Open Discussion Session

Wednesday, 3rd June

9:00 - Horst Puschmann (120 min)

A General Presentation of Quantum Crystallography Approaches

11:30 - Horst Puschmann (60 min)

Practical Applications QCr. Areas were QCr is giving new light!

12:30 - Horst Puschmann (60 min)

The use of Non-Spherical Form-Factors in structural Analysis

Free afternoon for study and culture

Thursday, 4th June

9:00 - Horst Puschmann & Pilar García (120 min)

Practical Session I: Dealing with Problematic Data/Structures

11:30 - Horst Puschmann & Fernando Lahoz (120 min)

Practical Session II: Dealing with Problematic Data/Structures - Absolute Structure

15:30 - Ilaria Gimondi & Andrew Peel (90 min)

Unlocking 3D Geometry: Search, Analyze, and Discover Structural Facts - New CSD Tools for Chemical Crystallography

17:30 - Horst Puschmann (90 min)

Practical Session III: Dealing with Problematic Data - Anomalous Scattering & Anharmonic Refinements

19:00 - Horst, Ilaria, Andrew and Pilar
Open Discussion Session

21:00 - All School Participants

Gala Dinner & more...

Friday, 5th June

09:00 - Andrew Peel and Ilaria Gimondi (60 min)

Exploring Structures & Voids in Porous Materials - How to Compare Crystal Structures

10:00 - Ilaria Gimondi & Andrew Peel (60 min)

Exploring Conformation and Non-Covalent Interactions - Interactions and Contacts in Crystals - I

11:30 - Andrew Peel and Ilaria Gimondi (60 min)

Exploring Conformation and Non-Covalent Interactions - Interactions and Contacts in Crystals - II

12:30 - Pilar García & Fernando Lahoz (60 min)

Last Opportunity to Finish your Structural Refinements - Structure Validation

13:30 - Fernando J. Lahoz & Pilar García
School Evaluation & Closing