



International AIC SCHOOL 2026

Bari, 20-23 July 2026

Department of Earth and Geoenvironmental Sciences, University of Bari, Italy

Scientific Programme

09:00 – 09:30 Registration

09:30 – 09:45 Welcome and Opening Remarks

Day 1 – From Diffraction to Structure Determination

Morning Session (Chair: Angela Altomare)

09:45 – 11:00 **Opening Lecture** — *The Phase Problem in Crystallography: A Challenge Worthy of a Nobel Prize* — **Carmelo Giacovazzo** (CNR-IC, Bari, Italy)

11:00 – 11:30 Coffee Break

11:30 – 12:30 *Structural Biology: An Amazing World* — **Doriano Lamba** (CNR-IC, Trieste, Italy)

12:30 – 14:00 Lunch

Afternoon Session (Chair: Cinzia Giannini)

14:00 – 15:00 *X-ray Diffraction: Principles and Experimental Techniques* — **Marco Mazzorana** (Diamond Light Source, Ltd., Didcot, UK)

15:00 – 16:00 *Solving Small-Molecule Structures Using Single-Crystal Diffraction* — **Anna Moliterni** (CNR-IC, Bari, Italy)

16:00 – 16:30 Coffee Break – Poster Session

16:30 – 17:30 *Structural Studies of Proteins: From Early Techniques to Modern Approaches* — **Dritan Siliqi** (CNR-IC, Bari, Italy)

17:30 – 18:10 *Advancing Crystallography Through Education and Infrastructure* — **Michele Zema** (Department of Earth and Geoenvironmental Sciences, University of Bari, Italy)

18:10 – 18:30 Short presentations of 5 minutes each

Day 2 – Structure Solution and Refinement: Methods and Software

Morning Session (Chair: Aurelia Falcicchio)

9:00 – 10:00 *X-ray Powder Diffraction for Structure Determination* — **Angela Altomare** (CNR-IC, Bari, Italy)

10:00 – 11:00 *Electron Diffraction in Structure Determination* — **Enrico Mugnaioli** (Department of Earth Sciences, University of Pisa, Italy)

11:00 – 11:30 Coffee Break – Poster Session

11:30 – 12:30 *SIR: Versatile Software for Single-Crystal Structure Solution* (Software presentation) — **Benedetta Carrozzini** (CNR-IC, Bari, Italy)

12:30 – 14:00 Lunch

Afternoon Session (Chair: Paolo P. Mazzeo)

14:00 – 15:00 *Olex2: An Easy-to-Use Program for Solving and Refining Small-Molecule Crystal Structures* (Software presentation) — **Florian Kleemiss** (Institut für Anorganische Chemie, RWTH Aachen, Germany)

15:00 – 16:00 *EXPO: Software for Structure Solution from Powder Diffraction Data* — **Corrado Cuocci** (CNR-IC, Bari, Italy) (Software presentation)

16:00 – 16:30 Coffee Break -Poster Session

16:30 – 17:30 *Structure Solution from Electron Diffraction Using SIR* — **Enrico Mugnaioli** (Department of Earth Sciences, University of Pisa, Italy), **Benedetta Carrozzini** (CNR-IC, Bari, Italy) (Software presentation)

17:30 – 18:30 *Software Packages for Biological Macromolecules Crystallography* — **Benny Danilo Belviso** (CNR-IC, Bari, Italy) (Software presentation)

Day 3 – Methods, Techniques and Computation in Crystallography

Morning Session (Chair: Michele Cianci)

09:00 – 10:00 *Diffraction from Advanced Materials and Nanostructures* — **Cinzia Giannini** (CNR-IC, Bari, Italy)

10:00 – 11:00 *Pair Distribution Function (PDF) Analysis: Methodology and Applications* — **Rocco Caliandro** (CNR-IC, Bari, Italy)

11:00 – 11:30 Coffee Break -Poster Session

11:30 – 12:30 *Linking Crystal Structure to Physical and Chemical Properties* — **Paolo P. Mazzeo** (Department of Chemical Sciences, Life Sciences and Environmental Sustainability, University of Parma, Italy)

12:30 – 14:00 Lunch

Afternoon Session (Chair: Marco Mazzorana)

14:00 – 15:00 *SUNBIM: A Software Suite for the Analysis of Nanoscale Materials* — **Francesco Scattarella** (CNR-IC, Bari, Italy) (Software Presentation)

15:00 – 16:00 *The Cambridge Structural Database (CSD) and Beyond* (Database Presentation) — **Andy Maloney** (CCDC, Cambridge, UK)

16:00 – 16:30 Coffee Break – Poster Session

16:30 – 18:00 *The Quantum ESPRESSO Package: DFT for Crystallography* (Software presentation) — **Davide Ceresoli** (Istituto di Scienze e Tecnologie Chimiche “G. Natta” – SCITEC-CNR, Milan, Italy)

18:00 – 18:30 Short presentations of 5 minutes each

20:00 Social Dinner

Day 4 – The Multifaceted and Interdisciplinary Character of Crystallography

Morning Session (Chair: Doriano Lamba)

9:00 – 10:00 *Crystallography of Natural Materials* — **Maria Lacalamita** (Department of Earth and Geoenvironmental Sciences, University of Bari, Italy)

10:00 – 11:00 *Crystallography for Pharmaceuticals* — **Fabia Gozzo** (Excelsus Structural Solutions, Villigen, Switzerland)

11:00 – 11:30 Coffee Break -Poster Session

11:30 – 12:30 *Ideal versus Real Crystals: Structural Defects* — **Giovanna Agrosi** (Department of Earth and Geoenvironmental Sciences, University of Bari, Italy)

12:30 – 14:00 Lunch

Afternoon Session (Chair: Sabrina Nazzareni)

14:00 – 15:00 *Artificial Intelligence for Crystal Structure Solution* — **Rocco Caliandro** (CNR-IC, Bari, Italy)

15:00 – 16:00 *Protein crystallization: understanding and tackling the bottleneck* — **Benny Danilo Belviso** (CNR-IC, Bari, Italy)

16:00 – 16:30 Coffee Break – Poster Session

16:30 – 17:10 *Modern Computational Tools for Drug Design* — **Vittoria Nanna** (CNR-IC, Bari, Italy)

17:10 – 17:40 *IUCr Journals: Disseminating High-Quality Crystallographic Research* — **Angela Altomare** (CNR-IC, Bari, Italy)

17:40 – 18:00 IUCr Journals Best Poster Prize and Closing Remarks
