EXPO&*more* International Workshop

Crystallographic Software for Powder Diffraction Data

30 September – 3 October 2019

Organized by the Institute of Crystallography (IC) – CNR Bari, Italy

The **EXPO&*more*** International Workshop is a four-day software fayre dedicated to the more recently developed versions of the open-source computer programs **EXPO, QUALX**, **OChemDb** and **RootProf**. The authors will expose the theoretical framework of the software, the program workflow, the latest developments and examples of application. The main aim of the workshop is to familiarize participants with the software.

Using diffraction data from polycrystalline materials, EXPO is devoted to crystal structure solution and QUALX to qualitative analysis for identification of the crystalline phase, one or more than one, contained in a compound. OChemDb is a web portal for assisting in the crystal-structure determination process by retrieving information, from a suitably designed database of crystal structures already solved, on bond distances, bond angles, torsion angles, atom types and space groups. RootProf is an interactive general-purpose tool for fast processing of measurements from in situ, in operando and/or multi-technique experiments.

Hands-on sessions will give participants the opportunity to use personally the packages under the supervision of the authors, as well as to process their own data.

Speakers

- Michele Saviano (Institute of Crystallography IC-CNR, Bari, Italy)
- Angela Altomare (Institute of Crystallography IC-CNR, Bari, Italy)
- Benny Danilo Belviso (Institute of Crystallography IC-CNR, Bari, Italy)
- Rocco Caliandro (Institute of Crystallography IC-CNR, Bari, Italy)
- Giovanni Cavallo (SUSPI, Switzerland)
- Nicola Corriero (Institute of Crystallography IC-CNR, Bari, Italy)
- Corrado Cuocci (Institute of Crystallography IC-CNR, Bari, Italy)
- Aurelia Falcicchio (Institute of Crystallography IC-CNR, Bari, Italy)
- Pietro Guccione (Electrical and Information Engineering Department of Politecnico of Bari, Italy)
- Akihiro Hymeda (Rigaku Company, Japan)
- Marco Milanesio (University of Eastern Piedmont, Alessandria, Italy
- Anna Moliterni (Institute of Crystallography IC-CNR, Bari, Italy)
- Rosanna Rizzi (Institute of Crystallography IC-CNR, Bari, Italy)
- Alessandro Zappi (University of Bologna, Bologna, Italy)

Program

Monday, 30th September 2019

8:30-13:00	Registration
9:30-9:45	**Michele Saviano** Director of Institute of Crystallography (IC)-CNR Welcome and opening session

EXPO Software

Chair: Rosanna Rizzi

9:45-10:30	**Angela Altomare** The structure solution process in the EXPO software
10:30-11:00	**Aurelia Falcicchio** Starting with EXPO
11:00-11:30	**Coffee break sponsored by Rigaku**
11:30-12:30	**Anna Moliterni** Indexing
12:30-13:00	**Akihiro Himeda** EXPO in the Rigaku software
13:00-14:30	**Lunch**

Chair: Angela Altomare

14:30-15:00	**Anna Moliterni** Space group determination

15:00-15:30	**Rosanna Rizzi** Full pattern decomposition
15:30-16:00	**Coffee break sponsored by Rigaku**
16:00-18:00	**Angela Altomare, Nicola Corriero, Corrado Cuocci,** **Aurelia Falcicchio, Anna Moliterni, Rosanna Rizzi** EXPO Computer session: Indexing and Space group determination
18:30-20:00	**Welcome party sponsored by Rigaku**

Tuesday, 1st October 2019

9:00-10:00	**Rosanna Rizzi** Reciprocal space methods solution
10:00-11:00	**Angela Altomare** Structure model optimization
11:00-11:30	**Coffee break**
11:30-13:00	**Corrado Cuocci** Direct space methods solution
13:00-14:30	**Lunch**
14:30-16:00	**Angela Altomare, Nicola Corriero, Corrado Cuocci,** **Aurelia Falcicchio, Anna Moliterni, Rosanna Rizzi** EXPO Computer session: Solution by Direct Methods and structure model optimization
16:00-16:30	**Coffee break**
16:30-18:30	**Angela Altomare, Nicola Corriero, Corrado Cuocci,** **Aurelia Falcicchio, Anna Moliterni, Rosanna Rizzi** EXPO Computer session: Structure model optimization and Rietveld refinement
18:30-	**Social event & Social dinner**

Wednesday, 2nd October 2019

9:00-9:30	**Corrado Cuocci** Rietveld refinement
9:30-10:30	**Angela Altomare, Nicola Corriero, Corrado Cuocci,** **Aurelia Falcicchio, Anna Moliterni, Rosanna Rizzi** EXPO Computer session: Rietveld refinement
10:30-11:00	**Coffee break**
11:00-13:00	**Angela Altomare, Nicola Corriero, Corrado Cuocci,** **Aurelia Falcicchio, Anna Moliterni, Rosanna Rizzi** EXPO Computer session: Direct space methods solution
13:00-14:30	**Lunch**

14:30-14:45	**Jasper Plaisier** Status of the diffraction beamlines at Elettra

QUALX Software

14:45-15:30	**Nicola Corriero** Qualitative phase analysis
15:30-16:15	**Giovanni Cavallo** Powder characterization by QUALX

16:15-16:45	**Coffee break**
16:45-18:30	**Angela Altomare, Nicola Corriero, Corrado Cuocci, Aurelia Falcicchio, Anna Moliterni, Rosanna Rizzi** QUALX Computer session

Thursday, 3rd October 2019

OCHEMDB Software

9:00-9:30	**Nicola Corriero** The OChemDb software
9:30-11:00	**Angela Altomare, Nicola Corriero, Corrado Cuocci,** **Aurelia Falcicchio, Anna Moliterni, Rosanna Rizzi** OChemDb Computer session
11:00-11:30	**Coffee break**

Thursday, 3rd October 2019

ROOTPROF Software

11:30-12:10	**Rocco Caliandro** RootProf: principles, workflow and new graphics user interface
12:10-12:40	**Pietro Guccione** New algorithms for fast extraction of information from in situ powder diffraction data
12:40-13:00	**Alessandro Zappi** Quantifying API polymorphs in solid formulations
13:00-14:30	**Lunch**

14:30-15:15	**Marco Milanesio**

	Monitoring in situ experiments with RootProf
15:15-15:45	**Benny Danilo Belviso** RootProf from theory to practice
15:45-16:15	**Coffee break**
16:15-18:30	**Rocco Caliandro, Benny Danilo Belviso** RootProf Computer session
18:30-19:00	**CLOSING SESSION**