

15th TOPAS Users' Meeting

August 28 - 30, 2024



Wednesday, 28.08.2024

- 12:00 – 13:00 Registration
- 13:00 – 13:10 Welcome
Arnt Kern, Bruker AXS, DE

Session 1: Analysis of large datasets – from PCs to the Cloud

- 13:10 – 13:35 Refining on 1000s of XRD patterns in one large refinement using TOPAS
Alan Coelho, Brisbane, AU
- 13:35 – 14:00 Using TOPAS in the Cloud
Peter Stephens, SUNY at Stonybrook, USA
- 14:00 – 14:25 PDF modelling of large supercells using cloud computing
Phil Chater, Diamond, UK
- 14:25 – 14:50 Using TOPAS to analyze XRD imaging data in 2 and 3 dimensions
David Wragg, University of Oslo, NO
- 14:50 – 15:15 Determination of the real space residual stress gradient in thin films using parametric refinement
Hugues Guerault, Bruker AXS, DE

Session 2: Line profile shapes and microstructure

- 15:15 – 16:00 Line profiles in TOPAS: basic and advanced modelling
Paolo Scardi, Uni Trento, IT
- 16:00 – 16:30 Coffee break
- 16:30 – 17:10 Modeling of incident-beam monochromators and k-edge absorption edges in powder diffraction
Marcus Mendenhall, NIST, US
- 17:10 – 17:35 Size anisotropy in Rietveld refinements
Dominique Ectors, Bruker AXS, DE
- 17:35 – 18:00 Morphological reconstruction from powder diffraction data
Peter Khalifah, Stony Brook University, USA

Session 3: New in TOPAS V7: GUI_Text

- 18:00 – 18:30 "GUI_Text": Useful applications in daily diffraction work
Dominique Ectors, Bruker AXS, DE
- 19:30 – 22:00 Reception at EXFORO Restaurant
Address: Prato della Valle 70/a

Thursday, 29.08.2024

Session 4: Structure Determination and Refinement

- 08:30 - 09:00 Methodologies for structure characterization: Strengths and Weaknesses
Rosanna Rizzi, Institute of Crystallography-CNR, IT
- 09:00 - 09:30 Powder diffraction is better than you imagined
Peter Khalifah, Stony Brook University, USA
- 09:30 - 10:00 Coffee break
- 10:00 - 10:25 Measurement Issues in Powder Diffraction, a NIST Perspective
Jim Cline, NIST, US
- 10:25 - 10:50 Inventory-taking of intensity contributions to a powder pattern
Robert Dinnebier, MPI Stuttgart, DE
- 10:50 - 11:15 Diffuse scattering in TOPAS and relation to total scattering methods
Paolo Scardi, Uni Trento, IT
- 11.15 - 11:40 Discrete structures and dual space refinements
Maxwell Terban, MPI Stuttgart, DE
- 11:40 - 12:05 Improving the results and accuracy of PDF refinements
Phil Chater, Diamond, UK
- 12:05 - 12:30 Symmetry Adapted Pair Distribution Function Analysis
Toby Bird, Diamond, UK
- 12:30 - 13:30 Lunch Break
- 13:30 - 13:55 Removing instrumental and emission profile effects – benefits of deconvolution for PDF analysis
Michael Evans, Bruker AXS, DE
- 13:55 - 14:20 Pushing laboratory PDF data quality – deconvolution or monochromatization?
Mirijam Zobel, RWTH Aachen, DE
- 14:20 - 14:45 Topas tips, tricks and tutorials: tracking transitions and transformations
John Evans, University of Durham, UK
- 14:45 - 15:10 Unravelling solid-solid phase transitions in coinage metal pyrazolates used for purification of ethylene
Peter Stephens, SUNY at Stonybrook, USA
- 15:10 - 15:35 Handling Non-Homogenous Samples – Refinement of a Li-Ion Battery
Dennis Becker, Bruker AXS, DE
- 15:35 - 16:00 Crystal structure determination of lead compounds and pharmaceuticals using X-ray powder diffraction
Fabio Furlan Ferreira, Universidade Federal do ABC, BR
- 16:00 - 16:30 Coffee break
- 16:30 - 16:55 Anisotropic displacement parameters of organic molecules from laboratory powder data?
Martin-Ulrich Schmidt, Uni Frankfurt, DE
- 16:55 - 17:20 Modelling pharmaceutical compounds from PDF Data using TOPAS
Fanny Costa, University of Leeds, UK
- 17:20 - 17:45 Structure determination of nano-crystalline organic compounds by a global fit to the PDF
Martin-Ulrich Schmidt, Uni Frankfurt, DE

Friday, 30.08.2024

Session 4: Structure Determination and Refinement, ctd.

- 08:30 – 09:00 XRPD and NPD data analysis of stacking faulted inorganic and organic materials using TOPAS - challenges and pitfalls
Sebastian Bette, MPI Stuttgart, DE
- 09:00 – 09:30 Understanding complex layered nanomaterials via XRD/PDF analysis
Scott Misture, Alfred University, USA
- 09:30 – 10:00 Coffee break
- 10:00 – 10:25 Supercell modeling for ordered alloys and oxides
Scott Misture, Alfred University, USA
- 10:25 – 10:50 Accurate peak broadening modelling for time-resolved in-situ ball milling reactions via synchrotron powder X-ray diffraction
Paolo Mazzeo, University of Parma, IT
- 10:50 – 11:15 Enigmatic Structure Property Behaviour in Bismuthate oxide ionic conductors
Dave Billing, University of the Witwatersrand, ZA

Session 5: Quantitative Phase Analysis

- 11.15 – 11:40 Quantitative phase analysis of commercial and recycled plaster
Fabio Furlan Ferreira, Universidade Federal do ABC, BR
- 11:40 – 12:05 X-rays vs. Neutrons in Quantitative Analysis; The Certification of SRMs 676b & 674c
Jim Cline, NIST, US
- 12:05 – 12:30 Wrap-Off
- 13:00 Lunch