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	More than just crystallography – Analysing large datasets using batch and parametric Rietveld refinement methods
	Michael Wharmby, Bruker AXS, DE

Session 2: Line profile shapes and microstructure

15:15 – 15:55	Line profiles in TOPAS: basic and advanced modelling
	Paolo Scardi, Uni Trento, IT
15:55 – 16:25	Coffee break
16:25 – 17:05	Modeling of incident-beam monochromators and k-edge absorption edges in powder diffraction
	Marcus Mendenhall, NIST, US
17:05 – 17:30	Size anisotropy in Rietveld refinements
	Dominique Ectors, Bruker AXS, DE
17:30 – 17:55	Morphological reconstruction from powder diffraction data
	Peter Khalifah, Stony Brook University, USA

Session 3: New in TOPAS V7: GUI_Text

17:55 – 18:05	Introduction to "GUI_Text"
	Arnt Kern, Bruker AXS, DE
18:05 – 18:30	"GUI_Text": Useful applications in daily diffraction work
	Dominique Ectors, Bruker AXS, DE
18:30 – 21:00	Reception at Padova Congress

Thursday, 29.08.2024

Session 4: Structure Determination and Refinement

08:30 - 08:55	Methodologies for structure characterization: Strengths and Weaknesses
	Rosanna Rizzi, Institute of Crystallography-CNR, IT
08:55 - 09:20	Powder diffraction is better than you imagined
	Peter Khalifah, Stony Brook University, USA
09:20 - 09:45	Measurement Issues in Powder Diffraction, a NIST Perspective
	Jim Cline, NIST, US
09:45 - 10:10	Inventory-taking of intensity contributions to a powder pattern
	Robert Dinnebier, MPI Stuttgart, DE
10:10 - 10:50	Coffee break
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 pharmaceutical compounds using TOPAS
	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	Structure determination of nano-crystalline organic compounds by a global fit to the PDF
	Robert Hühn, Uni Frankfurt, DE
17:20 - 17:45	Modelling pharmaceutical compounds from PDF Data using TOPAS
	Fanny Costa, Excelsus, CH

Friday, 30.08.2024

Session 4: Structure Determination and Refinement, ctd.

08:30 – 08:55	XRPD and NPD data analysis of stacking faulted inorganic and organic materials using TOPAS - challenges and pitfalls *Sebastian Bette, MPI Stuttgart, DE*
08:55 – 09:20	Understanding complex layered nanomaterials via XRD/PDF analysis *Scott Misture, Alfred University, USA*
09:20 – 09:45	Supercell modeling for ordered alloys and oxides *Scott Misture, Alfred University, USA*
09:45 – 10:10	Rietveld refinement with non-spherical atoms: A test of the BODD approach *Martin-Ulrich Schmidt, Uni Frankfurt, DE*
10:10 – 10:50	Coffee break
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 using TOPAS *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
12:30	Lunch