

Agenda

15th TOPAS Users Meeting

May 24 - May 26, 2020 - Šibenik, Croatia



Sunday, 24.05.2020

- 12:00 - 13:00 Registration and Lunch
- 13:00 - 13:15 Welcome and introduction
Arnt Kern, Bruker AXS, DE; Dragica Prill, Uni Frankfurt, DE

Session 1: Methodology

- 13:15 - 13:45 Optical aberrations from Johansson-type incident beam monochromators on Bragg-Brentano powder diffractometers, and their effect on high-resolution microstructure measurements
Marcus Mendenhall, NIST, US
- 13:45 - 14:15 TOPAS tools for line profile analysis.
Paolo Scardi, Uni Trento, IT
- 14:15 - 14:45 Modelling of anisotropic crystallite size and anisotropic microstrain
Dominique Ectors, Bruker AXS, DE
- 14:45 - 15:15 The robustness of Rietveld quantitative phase analysis
Matthew Rowles, Curtin University, AUS
- 15:15 - 16:00 Coffee break
- 16:00 - 16:30 Quantitative phase analysis by the Direct-Derivation Methodology
Matthew Rowles, Curtin University, AUS
- 16:30 - 17:00 How to use Mathematica for visualization of parameters in TOPAS
Robert Dinnebier, MPI Stuttgart, DE
- 17:00 - 17:30 Sequential and parametric refinements utilizing Topas and Matlab
Martin Rudolph, TU Freiberg, DE
- 17:30 - 18:00 Using the global optimization method in TOPAS for solving the indexing problem, unsolved mathematical problems and Sudoku
Martin Etter, DESY, Hamburg, DE
- 19:00 Reception

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Monday, 25.05.2020

Session 1: Methodolgy, ctd.

- 08:30 - 09:00 Big-boxes in the cloud: PDF modelling of large supercells using cloud computing
Phil Chater, Diamond, UK
- 09:00 - 09:30 Technical advances and new reconstruction approaches for X-ray diffraction computed tomography data
Antonis Vamvakeros, University College London, UK
- 09:30 - 10:00 PDF generation using TOPAS: Improving the precision of PDF data via deconvolution
Phil Chater, Diamond, UK
- 10:00 - 10:30 Pair distribution function analysis in the home laboratory
Michael Evans, Bruker AXS, DE
- 10:30 - 11:00 Coffee

Session 2: Applications

- 11:00 - 11:30 Diffraction tomography of operating catalytic materials
Dorota Matras, University of Manchester and Finden Ltd., UK
- 11:30 - 12:00 Exploring the chemistry of fast lithium ion battery charging with time and space resolved operando XRD
David Wragg, University of Oslo, NO
- 12:00 - 12:30 Characterizing phase development for micronization and amorphization of an active pharmaceutical ingredient for HIV treatment
Maxwell Terban, MPI Stuttgart, DE
- 12:30 - 14:00 Lunch
- 14:00 - 14:30 Structure refinement by PDF fit, Rietveld refinement and lattice-energy minimisations of monomethyl-quinacridone $C_{21}H_{14}N_2O_2$
Martin-Ulrich Schmidt, Uni Frankfurt, DE
- 14:30 - 15:00 Sequential Refinement of time-resolved XRPD measurements using TOPAS.
Luzia Germann, McGill University, CA
- 15:00 - 15:30 Symmetry mode analysis of phase transformations of framework structures during ion exchange from HR synchrotron data
Scott Misture, Alfred University, USA
- 15:30 - 16:00 Thermal motion of crystalline isopropyl alcohol - beating over-parameterization into submission
Pamela Whitfield, Excelsus, CH
- 16:00 - 16:30 Coffee
- 16:30 - 17:00 Fullerene polymers revisited
Peter Stephens, SUNY at Stonybrook, USA
- 17:00 - 17:30 H atom positions of medium-sized organic molecules from laboratory powder data?
Martin-Ulrich Schmidt, Uni Frankfurt, DE
- 17:00 - 17:30 Manganese cyanide tinkertoys
Peter Stephens, SUNY at Stonybrook, USA

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Tuesday, 26.05.2020

Session 2: Applications, ctd.

- 09:00 - 09:30 WPPM-TOPAS in the development of creep-strength enhanced ferritic steels
Paolo Scardi, Uni Trento, IT
- 09:30 - 10:00 Simple modeling of complex local structure distortions in battery cathodes using TOPAS
Peter Khalifah, Stony Brook University, USA
- 10:00 - 10:30 Real and reciprocal space analysis of layered oxides and exfoliated 2-D materials
Scott Mixture, Alfred University, USA
- 10:30 - 11:00 Microstructural characterization of stacking faulted NCA-/NCM-battery material precursors and of iridate catalysts of oxygen evolution reactions by automated, multidimensional grid search routines
Sebastian Bette, MPI Stuttgart, DE
- 11:00 - 11:30 Coffee
- 11:30 - 12:00 Quantification of Li loss from battery cathode materials with parts-per-ten-thousand sensitivity by powder diffraction
Peter Khalifah, Stony Brook University, USA
- 12:00 - 12:30 Anisotropic thermal expansion in multifunctional materials
Gianpiero Gallo, MPI Stuttgart, DE
- 12:30 - 13:00 Decomposition yields something new: Structure elucidation of corrosion phases found on museum exhibits.
Sebastian Bette, MPI Stuttgart, DE
- 13:00 Wrap-Up
Arnt Kern, Bruker AXS, DE; Dragica Prill, Uni Frankfurt, DE