CanSAS 2023

Collective action for nomadic Small Angle Scatterers

ILL/ESRF, Grenoble: 16 - 18 October 2023

All talks will take place in the ESRF auditorium

Monday 16th October

11:00-12:00	**Arrivals + Registration : ESRF entrance Hall** Please collect your name badge that can be shown to pay for your lunch (non ILL/ESRF staff only) Please also install your poster on the poster boards.	
12:00-13:30	Lunch (Canteen) *Tables reserved downstairs at the back of the canteen, coffee included*	
13.30-14:00	Introductory words from ILL Science Director and ESRF Director of Research	Jacques JESTIN (Theyencheri Narayanan on behalf of Michael Krisch)
Machine learning based SAS analysis / Chair of session : Sylvain Prévost /Theyencheri Narayanan 14:00 – 16:00		
14:00-14:30	The Autonomous Formulation Lab: Industrial Formulation Optimization Combining SAS & ML	Tyler MARTIN *(NIST, USA)*
14:30-15:00	Machine Learning for SAS: A Lay of the Land – Pitfalls, Beartraps and All	Tim SNOW *(Diamond Light Source, UK)*
15:00-15:30	Inferring Lyotropic Phase Topology through Scattering using Deep Learning	Wei-Ren CHEN *(Oak Ridge National Laboratory, USA)*
15:30-16:00	Machine-learning-assisted Analysis of Small Angle X-ray Scattering	Yu SHEN *(RISE Research Institute, Sweden)*
16:00-16:30	Coffee Break (ESRF Entrance Hall) *** **GROUP PHOTO** ***	
Automation & software / Chair of session : Nick Terrill (Diamond, U.K) 16:00-18:00		
16:30-17:00	Autonomous Materials Discovery using X-ray Scattering	Kevin YAGER *(Brookhaven National Laboratory, USA)*
17:00-17:20	A holistic experiment chain for scattering-powered materials science Investigations	Brian Richard PAUW *(BAM Berlin)*
17:20-17:40	SAXSutilities: a graphical user interface for processing and analysis of Small-Angle X-ray Scattering data	Peter BOESECKE *(ESRF)*
17:40-18:00	Cross-Facility Workflow Development for Live Analysis and Visualization	Wiebke KOEPP *(ALS, Lawrence Berkeley National Lab, USA)*
18.00 →	Poster session and Discussion with Wine and Cheese	

Tuesday 17th October

SAS based imaging / Chair of session : Florian Meneau (SIRIUS) 9:00 – 11:00		
09:00-09:30	Real Space and Reciprocal Space Mapping in Small Angle	Byeongdu LEE *(APS, Argonne National Laboratory, USA)*
09:30-10:00	Coherent diffraction imaging at the ESRF EBS - progress and challenges	Yuriy CHUSHKIN *(ESRF)*
10:00-10:30	Coherent Surface Scattering in Grazing Incidence and Reflection: Advancements and Challenges	Jin WANG *(APS, Argonne National Laboratory, USA)*
10:30-11:00	Nerve Fibers And Myelin Assembly In A Mouse Brain Section	Henrich FRIELINGHAUS *(Fz Jülich, Germany)*
11:00 – 11:30	Coffee Break (ESRF Entrance Hall)	
Emerging sample-environments and methods / Chair of session : U-Ser Jeng (NSRRC) 11:30 – 12:50		
11:30-12:00	BioSAXS in the Age of High-Resolution Structural Biology: Advancing with Innovative Sample Environments	Clement BLANCHET *(EMBL-Petra 3, Hamburg Germany)*
12:00-12:30	Advanced SANS sample environments	Anne MARTEL *(ILL)*
12:30-12:50	BioSAXS Sample Environments at TPS 13A	Orion SHIH *(National Synchrotron Radiation Research Center, Taiwan)*
12:50 - 14:00	Lunch (Canteen) *Tables reserved downstairs at the back of the canteen, coffee included*	
Needs and developments of analysis programs / Chair of session : Adrian Rennie (Uppsala) 14:00 – 16:00		
14:00 – 14:30	Challenges and Opportunities in Hierarchical Modeling of X-ray Scattering Data from Complex Structures	Uri RAVIV *(Hebrew University of Jerusalem, Israel)*
14:30 - 15:00	Combining SAXS with molecular dynamics simulations for a quantitative and atomic view on the protein hydration shell	Jochen HUB *(Saarland University, Germany)*
15:00-15:30	The state of the art of GENFIT, an advanced software for the analysis of SAS data	Francesco SPINOZZI *(Polytechnic University of Marche, Italy)*
15:30-16:00	Future developments in SasView – the challenge of meeting community Aspirations	Wojciech POTRZEBOWSKI *(ESS Sweden)*
16:00 – 16:30	Coffee Break (ESRF Entrance Hall)	
Simultaneous modeling: needs, pitfalls, solutions / Chair of session : Judith Houston (ESS) 16:30 -18:10		
16:30- 17:00	Pitfalls and how to avoid them when simultaneously modelling small-angle neutron and X-ray scattering data	Jan Skov PEDERSEN *(Aarhaus University, Denmark)*
17:00-17:30	A seamless model for seamless scattering data including molecular and colloidal scales in wood cell walls	Yoshiharu NISHIYAMA *(CERMAV, France)*
17:30-17:50	Reflection, refraction, and scattering from liquid foams	Leonardo CHIAPPISI *(ILL)*
17:50-18:10	BornAgain - open-source cross-platform software to simulate & fit GISAS & reflectometry	Mikhail SVECHNIKOV *(Fz Jülich, Germany)*
18:10-19:30	**Discussions led by Peter Bösecke, Charles Dewhurst, Theyencheri Narayanan and Sylvain Prévost**	
20:30 →	Dinner at Brasserie des Antiquaires, 7 Rue de la Paix, 38000 Grenoble	

Wednesday 18th October

	Open access / databases / collaborations between facilities/ Chair of session : Charles Dewhurst (ILL) 9:00 – 10:30	
09:00-09:30	Enhancing collaboration between facilities world wide	Adrian RENNIE *(Uppsala University, Sweden)*
09:30-10:00	The Small Angle Scattering Biological Data Bank (SASBDB) - more than a FAIR repository	Cy JEFFRIES *(EMBL Hamburg, Germany)*
10:00-10:30	Report from the CanSAS working groups	Stephen KING *(ISIS, UK)*
10:30 – 11:00	Coffee Break and Poster Removal (ESRF Entrance Hall)	
11:00-12:00	Discussions	
12:00 - 13:00	CanSAS 2024 Wrap-up	U-Ser Jeng *(NSRRC, Taiwan)*
13:00 →	Lunch (Canteen) *Tables reserved downstairs at the back of the canteen, coffee included*	

Many thanks to the support from: