

# Online Workshop on ePDF 1-2 September 2021



## Program

All times are given in CET (Central European Time)

Wednesday, 1<sup>st</sup> of September

	<b>Introduction to (e)PDF, data collection, processing, applications</b> <i>Chair: Antonietta Guagliardi</i>
9:00 - 9:30 (30 min)	<b>Kirsten Jensen</b> , University of Copenhagen, <a href="mailto:kirsten@chem.ku.dk">kirsten@chem.ku.dk</a> Introduction into PDF
9:30 - 9:50 (20 min)	<b>Tatiana Gorelik</b> , Ulm University, <a href="mailto:Tatiana.gorelik@uni-ulm.de">Tatiana.gorelik@uni-ulm.de</a> Specialities of electron scattering regarding PDF
9:50 - 10:10 (20 min)	<b>Xiaoke Mu</b> , KIT, Karlsruhe, <a href="mailto:xiaoke.mu@kit.edu">xiaoke.mu@kit.edu</a> ePDF mapping for revealing atomic bonds in amorphous nanoscale phases
10:10 - 10:30 (20 min)	<b>Martin U. Schmidt</b> , University of Frankfurt am Main, <a href="mailto:M.Schmidt@chemie.uni-frankfurt.de">M.Schmidt@chemie.uni-frankfurt.de</a> Applications of X-ray PDF
10:30 - 10:45	<i>Virtual coffee break</i>
	<b>Data processing for ePDF calculation – software</b> <i>Chair: Tatiana Gorelik</i>
10:45 - 11:15	<b>Partha Das</b> , NANOMEGAS, <a href="mailto:partha@nanomegas.com">partha@nanomegas.com</a> Data Analysis Software for Amorphous and Nanocrystalline Material in TEM. ePDF suite
11:15 - 11:45	<b>Cheuk-Wai Tai</b> , Stockholm University, <a href="mailto:cheuk-wai.tai@mmk.su.se">cheuk-wai.tai@mmk.su.se</a> SUEPDF
11:45 - 12:15	<b>Tim Petersen</b> , Monash University, <a href="mailto:timothy.petersen@monash.edu">timothy.petersen@monash.edu</a> RDFTools
12:15 - 13:45	<i>Lunch break</i>
13:45 - 14:15	<b>Janos Labar</b> , Center for Energy Research, Budapest, <a href="mailto:labar.janos@energia.mta.hu">labar.janos@energia.mta.hu</a> ProcessDiffraction
14:15 - 14:45	<b>Janaki Shanmugam</b> , IMRE, Singapore, <a href="mailto:Janaki_Shanmugam@imre.a-star.edu.sg">Janaki_Shanmugam@imre.a-star.edu.sg</a> eRDF Analyser (Konstantin Borisenko)
	<b>Refinement /modelling of structures</b> <i>Chair: Reinhard Neder</i>
14:45 - 15:15	<b>Ana-Suncana Smith</b> , University of Erlangen-Nuremberg, <a href="mailto:smith@physik.uni-erlangen.de">smith@physik.uni-erlangen.de</a> Molecular Dynamics
15:15 - 15:30	<i>Virtual coffee break</i>
15:30 - 16:00	<b>Emil Bozin</b> , Brookhaven Natl Lab, <a href="mailto:bozin@bnl.gov">bozin@bnl.gov</a> PDFGui - small box platform for modelling PDF data
16:00 - 16:30	<b>Matt Tucker</b> , <a href="mailto:tuckermg@ornl.gov">tuckermg@ornl.gov</a> RMC Profile
16:30 - 17:00	<b>Paul Voyles</b> , University of Wisconsin-Madison, <a href="mailto:paul.voyles@wisc.edu">paul.voyles@wisc.edu</a> Fluctuation Electron Microscopy

Thursday, 2nd of September

	<p><b>Amorphous, nanocrystalline and disordered structures</b>  <b>Chair: Tatiana Gorelik</b></p>
9:00 - 9:30	<p><b>Matthew Cliffe</b>, School of Chemistry, University of Nottingham,  <a href="mailto:pczmjc1@exmail.nottingham.ac.uk">pczmjc1@exmail.nottingham.ac.uk</a>          How defects show up in powder /PDF</p>
9:30 - 10:00	<p><b>Reinhard Neder</b>, University of Erlangen-Nuremberg, <a href="mailto:reinhard.neder@fau.de">reinhard.neder@fau.de</a>          DISCUS</p>
10:00 - 10:30	<p><b>Tim Petersen</b>, Monash University, <a href="mailto:timothy.petersen@monash.edu">timothy.petersen@monash.edu</a>          Hybrid Reverse Monte Carlo modelling</p>
10:30 - 10:45	<p><i>Virtual coffee break</i></p>
	<p><b>Working in reciprocal space: Debye scattering technique, Debussy Suite, Applications</b>  <b>Chair: Reinhard Neder</b></p>
10:45 - 11:15	<p><b>Antonietta Guagliardi</b>, Institute of Crystallography, CNR, Italy          The Debye Scattering Equation Method for exploring the nanocrystals world  <a href="mailto:antonella.guagliardi@ic.cnr.it">antonella.guagliardi@ic.cnr.it</a></p>
11:15 - 11:45	<p><b>Ruggero Frison</b>, University of Zurich          Debussy Suite  <a href="mailto:ruggero.frison@physik.uzh.ch">ruggero.frison@physik.uzh.ch</a></p>
11:45 - 13:15	<p><i>Lunch break</i></p>
	<p><b>Texture in PDF</b>  <b>Chair: Antonietta Guagliardi</b></p>
13:15 - 13:30	<p><b>Tatiana Gorelik</b>, Ulm University          Texture in ED  <a href="mailto:Tatiana.gorelik@uni-ulm.de">Tatiana.gorelik@uni-ulm.de</a></p>
13:30 - 14:00	<p><b>Ruggero Frison</b>, University of Zurich          Texture corrections in DSE and PDF  <a href="mailto:ruggero.frison@physik.uzh.ch">ruggero.frison@physik.uzh.ch</a></p>
14:00 - 14:30	<p><b>Reinhard Neder</b>, University of Erlangen-Nuremberg          DSE / PDF  <a href="mailto:reinhard.neder@fau.de">reinhard.neder@fau.de</a></p>
14:30 - ...	<p>Discussions</p>