PROGRAM OF THE 7TH REVERSE MONTE CARLO CONFERENCE

The first 30 years of Reverse Monte Carlo Modelling

20-22 September, 2018, Budapest

THURSDAY (20TH SEPTEMBER)

8:50	***László Pusztai*** *Introduction and Welcome*	*Wigner RCP (Hungary)*
9:00	**David Keen** Thirty years of RMC: An introduction and review of recent developments	ISIS (UK)
9:30	**Pál Jóvári** Short range order in covalent glasses - problems and possible solutions	Wigner RCP (Hungary)
10:00	**Matt Tucker** ((… crystals by RMC…))	SNS/ORNL (USA)
10:30	**COFFEE**	
11:00	**Ildikó Pethes** On the structure of highly concentrated aqueous lithium chloride solutions from a combination of RMC and MD techniques and 29 interatomic potential models	Wigner RCP (Hungary)
11:20	**Tom Farmer** Tailoring molecular potentials for dynamics using quasi-elastic neutron scattering	ISIS (UK)
11:40	**Szilvia Pothoczki** Temperature-induced changes in the hydrogen-bond network of isopropanol-water mixtures at low isopropanol concentration	Wigner RCP (Hungary)
12:00	**Joe Paddison** Understanding Spin Liquids using RMC Refinement	University of Cambridge (UK)
12:20	**Mark Wilkinson** Analysis of Rhenium Trioxide as a model for using a phonon-based displacement methodology in RMC	Queen Mary University of London (UK)
12:40	**LUNCH**	
14:10	**Janis Timoshenko** Deciphering the structure of metallic nanoparticles using reverse Monte Carlo method, molecular dynamics and machine learning	Stony Brook University, NY, USA

14:30	**Helen Playford** Insights into Stacking Disorder in Ice I using Pair Distribution Functions	ISIS (UK)
14:50	**Harry Geddes** Compositional inhomonogeity in mixed-metal MOFs	University of Oxford (UK)
15:10	**Phillip Maffettone** Amorphous zeolitic imidazolate frameworks with D_{4h} local symmetry	University of Oxford (UK)
15:30	**COFFEE and POSTERS**	
16:20	**Nick Funnell** High-pressure total scattering at ISIS	ISIS (UK)
16:40	**Karen Appel** New perspectives for high energy density science studies using free electron laser (FEL) light source	European XFEL (Germany)
17:00	**Gyula Faigel** The possibility of structural studies by a single XFEL pulse	Wigner RCP (Hungary)
17:30	**END**	

FRIDAY (21TH SEPTEMBER)

9:00	**Andrew Goodwin** When does RMC work? When does RMC fail? (A personal perspective)	University of Oxford (UK)
9:30	**Martin Dove** Neutron total scattering studies of three multiferroic crystals	Queen Mary University of London (UK)
10:00	**Alexei Kuzmin** Disorder effects in EXAFS spectra: molecular dynamics vs reverse Monte Carlo simulations	University of Latvia (Riga, Latvia)
10:20	**Angela Trapananti** Structural refinement of molecular and condensed systems by RMC-GNXAS: recent advances and applications	University of Camerino (Italy)
10:40	**COFFEE**	
11:10	**Karel Saksl** Atomic structure of Ca-based metallic glasses	Slovak Academy of Sciences (Slovakia)
11:30	**Shinya Hosokawa** Partial structures of the traditional bulk metallic glass $Pd_{40}Ni_{40}P_{20}$	Kumamoto University (Japan)
11:50	**Stefan Michalik** Binary Cu-Hf metallic glasses investigated by the reverse Monte Carlo simulation and Voronoi analysis	Diamond Light Source (UK)

12:10	**Yohei Onodera** Modification of Phosphate Network in binary zinc phosphate glass	University of Kyoto (Japan)
12:30	**LUNCH**	
14:00	**Wojciech Slawinski** RMCProfile7: Reverse Monte Carlo program for modelling of multiphase systems	ISIS (UK)
14:20	**Guanqun Cai** Experiments with RMCprofile 7: multiphase RMC	Queen Mary University of London (UK)
14:40	**Victor Krayzmann** Combined-technique structure refinements in RMCProfile	NIST (USA)
15:00	**Tomotaka Nakatani** Evaluation of dispersion state of silica particles in rubber during elongation using RMC modelling	RIKEN/Spring-8 (Japan)
15:20	**Rupert Tscheließnig** How proteins scatter – fractal aspects	Universitaet für Bodenkultur (Austria)
15:40	**COFFEE and POSTERS**	
16:20	**Naoto Kitamura** Local Structure Analysis on $Na_{0.5}Bi_{0.5}TiO_3$-Based Materials with Perovskite Structure	Tokyo University of Science (Japan)
16:40	**László Temleitner** Studying the structure of Li-salts using molecular dynamics and Reverse Monte Carlo methods	Wigner RCP (Hungary)
17:00	**Jiaxun Liu** Local structure of lead halide perovskites for photovoltaic applications	Queen Mary University of London (UK)
17:20	**Marshall McDonnell** Guest-Host Interactions in Mixed CH_4–CO_2 Hydrates: Neutron total scattering and computational modeling	ORNL/SNS
17:40	**END**	

SATURDAY (22TH SEPTEMBER)

9:00	**Markus Winterer** Dopant Position in Inorganic Semiconductor Nanoparticles from Reverse Monte Carlo (RMC) analysis of Extended X-ray Absorption Fine Structure (EXAFS) Spectra	University of Duisburg-Essen (Germany)
9:20	**Inga Jonane** Treatment of disorder in XANES by RMC simulations	University of Latvia (Riga, Latvia)
9:40	**Lei Tan** RMC for nanoclusters	Queen Mary London (Uk)

10:00	**Andris Anspoks** Reverse Monte Carlo CuO local structure studies across magnetic transitions (T = 10 - 300K) from EXAFS data	University of Latvia (Riga, Latvia
10:20	**COFFEE**	
10:50	**Lewis Owen** Local effects in crystalline alloys using RMC	ISIS (UK)
11:10	**Hiroki Yamada** Structural Evolution of Amorphous Precursors towards Zeolites Visualized by in-situ Relative PDF Approach	University of Tokyo (Japan)
11:30	**Benjamin Klee** Molecular RMC simulation on amorphous [(PhSn)4S6] without using potentials	Marburg University (Germany)
11:50	**Makina Saito** Microscopic Structure and Dynamics in Ionic Glass Ca0.4K0.6(NO3)1.4: Quasi-Elastic Gamma-Ray Scattering and X-Ray Diffraction Studies	University of Kyoto (Japan)
12:10	**… ??? …** *Closing comments and Summary: the next 30 years of RMC modelling (?)*	
12:30	**LUNCH**	