

TIMETABLE OF THE 6TH REVERSE MONTE CARLO CONFERENCE

TIME *THURSDAY (17TH SEPTEMBER)*

8:55	László Pusztai	Wigner RCP (Hungary)	Introduction and Welcome
9:00	David Keen	ISIS (UK)	The first 27 years of reverse Monte Carlo
9:30	Sylvia McLain	Oxford (UK)	Probing biomolecular structure in aqueous solution: Insights from neutron diffraction and computation
10:00	Nick Funnell	Oxford (UK)	RMC and the nanoscale
10:30	COFFEE		
11:00	Lewis Owen	Cambridge/ISIS (UK)	Short range order in alloys
11:20	Yohei Onodera	Kyoto (Japan)	Reverse Monte Carlo methods for superionic conductors
11:40	Peter Thygesen	Oxford (UK)	Small displacements, big effect: correlated orbital disorder drives spin-glass state in Y ₂ Mo ₂ O ₇
12:00	Kaustuv Datta	Hamburg (Germany)	Local structures of perovskite based ferroelectric solid solutions containing morphotropic phase boundary
12:20	Alistair Overy	Oxford (UK)	Disorder-phonon coupling in crystal-like aperiodic solids
12:40	LUNCH		
14:10	Orsolya Gereben	Wigner RCP (Hungary)	Characterization of the hydrogen-bonded network in ethanol-water mixtures
14:30	Koji Ohara	Spring-8 (Japan)	Liquid structure of the electrolyte material Li/Mg/Cs-TFSA molten salt
14:50	Szilvia Pothoczki	Wigner RCP (Hungary)	Linearity vs. tetrahedrality in acetonitrile molecular liquid
15:10	Anthony E. Phillips	Queen Mary London (UK)	Phase transitions in molecule-containing crystals
15:30	COFFEE and POSTERS		
16:20	Imre Bakó	Natural Sciences Research Centre (Hungary)	A new approach to the determination of the uncertainty on neutron diffraction experiments with isotopic substitution
16:40	Arkadiy Simonov	Oxford (UK)	3D-ΔPDF + RMC: a microscopic model of orientational frustration in an organic single crystal
17:00	László Temleitner	Wigner RCP (Hungary)	H-bonded and non-H bonded liquids: removing the incoherent scattering of 1H polarized neutrons
17:20	END		

TIME**FRIDAY (18TH SEPTEMBER)**

9:00	Alan Soper	ISIS (UK)	Recent developments in EPSR
9:30	Andrew Goodwin	Oxford (UK)	RMC for magnets
10:00	László Pusztai	Wigner RCP (Hungary)	Determining the structure of molecular liquids by combining molecular dynamics and RMC
10:30	COFFEE		
11:00	Matt Tucker	ISIS/DIAMOND (UK)	The new XPDF beam line at Diamond
11:20	Luis Rodríguez Palomino	ILL (France)	The structure factor of liquid propanol studied by polarized neutron diffraction and RMC
11:40	Viviana Cristiglio	ILL (France)	Structure investigation of molecular liquids and liquid solutions by small angle neutron scattering
12:00	Vicente Sanchez Gil	CSIC Madrid (Spain)	N-RMC method: Reverse Monte Carlo modeling in confined systems
12:20	Serena Maugeri	Queen Mary London (UK)	Modelling nanoparticles structure using PDFgui and RMCprofile
12:40	LUNCH		
14:10	Rupert Tscheließnig	Bodenkultur Uni (Austria)	Interfacial forces of proteins and surfaces
14:30	Nicola Steinke	Oxford (UK)	Atomic level insights into urea induced protein unfolding
14:50	Will Fletcher	Oxford (UK)	A Bayesian route to protein structure without crystals
15:10	Andrew Johnston	Oxford (UK)	The Atomic Structure of Pharmaceuticals in Solution: Penetrating the Blood-brain Barrier
15:30	COFFEE and POSTERS		
16:20	Janis Timoshenko	Latvia Uni (Latvia)	Reverse Monte Carlo/evolutionary algorithm approach for the analysis of EXAFS data from distant coordination shells of crystalline materials
16:40	Helen Playford	ISIS (UK)	How long is long enough?
17:00	Phillip Tucciarone	Oxford (UK)	NTE, spaghetti dynamics, and hydration-driven volume collapse in ZrW ₂ O ₈
17:20	END		

TIME**SATURDAY (19TH SEPTEMBER)**

9:00	Pál Jóvári	Wigner RCP (Hungary)	Short range order in CuZr based metallic glasses
9:20	Ildikó Pethes	Wigner RCP (Hungary)	Chemical order in chalcogenide glasses
9:40	Ilkyoung Jeong	Pusan (Korea)	Separation of thermal disorder from static displacements in RMC modeling
10:00	Juan Du	Queen Mary London (UK)	After RMC refinement: new tools for analyzing refined configurations (with case study BiFeO ₃)
10:20	COFFEE		
10:50	Mona Bahout	Rennes (France)	Stability under hydrogen and humid conditions of potential SOFC electrodes investigated by high-

			temperature in situ neutron powder diffraction
11:10	Huw Marchbank	UC London (UK)	Understanding how different synthetic procedures influence the short, medium and long range atomic arrangement in ceria
11:30	Giles Flowitt-Hill	Edinburgh/ISIS (UK)	Local order of small organic molecules in crystals
11:50	Dominic Carter	Queen Mary London (UK)	The local structure of beta-cristobalite as a composite of low symmetry domains
12:10	<i>László Pusztai</i>	<i>Wigner RCP (Hungary)</i>	<i>Closing comments and Summary</i>
12:30	LUNCH		