## Program QENS/WINS 2016

Monday,	5 <sup>th</sup> September 201	.6
09:00	Registration	
12:00	Lunch Break	
		Thomas Frederking (Helmholtz-Zentrum Berlin)
13:00	Welcome	Margarita Russina (Helmholtz-Zentrum Berlin)
		Oliver Delaire (Duke University)
		Phonon Scattering Processes in Thermoelectrics Investigated with Neutron Scattering
	PlenaryTalk:	and
13:30	New Challenges	First-Principles Simulations
	Materials for ener	gy conversion
		Christopher Stock (University of Edinburgh)
14:15	Invited Talk	Soft excitations in perovskite piezoelectrics and photovoltaics
		Florian Pforr (Technische Universität Darmstadt)
14:45		Local diffusion and critical scattering in a lead-free relaxor ferroelectric
		Sanghamitra Mukhopadhyay (STFC Rutherford Appleton Laboratory)
		Application of ab-initio Molecular Dynamics in Modelling of Quasielastic Neutron
15:05		Scattering on Functional Materials
15:25	Coffee Break	
	Materials for ener	gy storage
		Stephane Rols (Institut Laue-Langevin)
15:55	Invited Talk	Hydrogen motions in defective graphene: the role of surface defects
		Alexander J. O'Malley (University College London)
16:25		Sorbate Dynamics in Zeolite Catalysts: Tandem QENS and Simulation Studies
		Ian Silverwood (STFC Rutherford Appleton Laboratory )
16:45		Investigation of Zeolite Pore Blocking with QENS
		Heisi Kurig (University of Tartu)
		The pore size and shape of nanoporous carbons and influence of porosity on
17:05		hydrogen adsorption kinetics
		Iain Hitchcock (Johnson Matthey Technology Centre)
17:25		Measuring the diffusion of ammonia in zeolite NOx emissions control catalysts
		Wiebke Lohstroh (Technische Universität München)
17:45		Hydrogen dynamics in $\beta$ -Mg(BH <sub>4</sub> ) <sub>2</sub> on the picosecond timescale
18:05	End	

Tuesday, 6 <sup>th</sup> September 2016		
	Materials for ener	gy conversion
	Plenary Talk:	Piers R. F. Barnes (Imperial College London)
09:00	New Challenges	Movement and disorder in methylammonium lead halides for solar cells
		David Djurado (CNRS )
		Lattice and local dynamics in disordered solid materials for organic and hybrid
09:45	Invited Talk	(opto)electronic applications
		Michael Koza (Institut Laue-Langevin)
		Relaxation Processes in Thermoelectric Materials
10:15	Invited Talk	

10:45	Coffee Break	
	Ionic and proton o	conducting systems
		Kazuhiro Mori (Kyoto University)
		Direct observation of fast lithium-ion diffusion in a superionic conductor: $Li_7P_3S_{11}$
11:00	Invited Talk	metastable crystal
		Fanni Juranyi (Paul Scherrer Institut)
11:30		Ionic diffusion in battery cathods, e.g. Na <sub>0.7</sub> CoO <sub>2</sub>
		Daria Noferini (Chalmers University of Technology )
		Proton dynamics in hydrated acceptor-doped barium zirconates investigated with
11:50		neutron spectroscopy
		Artur Braun (Empa)
12:10		On the metafunction of protons in ceramic electrolytes
12:30	Lunch	
	Electrolytes and ic	onic liquids
		Natalie Malikova (University Pierre and Marie Curie)
		Interactions in polyelectrolyte solutions probed by neutron scattering: charge,
13:30	Invited Talk	hydrophobicity and ion-specific effects
		Eugene Mamontov (Oak Ridge National Laboratory)
14:00	Invited Talk	Microscopic Dynamics of Confined Electrolytes for Energy Storage Applications
		Antonio Benedetto (Paul Scherrer Institute )
		Biomolecules, Water and Room-Temperature Ionic Liquids: a Neutron Scattering and
14:30		Computational study
		Tatsiana Burankova (Paul Scherrer Institute)
		Dynamic Heterogeneity and Flexibility of the Alkyl Chain in Pyridinium-Based Ionic
14:50		Liquids
		Jean-Marc Zanotti (LLB (CEA-CNRS))
15:10		Ionic liquids in bulk and under 1D nanometric confinement: a multiscale analysis
		Tommy Hofmann (Helmholtz-Zentrum Berlin)
		Quasi-elastic neutron scattering study of a room-temperature ionic liquid confined in
15:30		nanoporous carbon
15:50	Postersession incl. R	Refreshments and Snacks
18:00	End	

## Wednesday, 7<sup>th</sup> September 2016 Fuel Cells Jan-Patrick Melchior (Max-Planck-Institut für Festkörperforschung) From the unique proton diffusion in neat phosphoric acid to fuel cell membranes – A QNS and NMR study of model systems unveiling chemical influences on proton 09:00 Invited Talk Micolas Martinez (CNRS) 09:30 Nanoscale water dynamics in operando fuel cells 09:50 Oxana Ivanova (Jülich Centre for Neutron Science) Proton dynamics in high temperature polymer electrolyte fuel cell membranes

		Marina Khaneft (Jülich Centre for Neutron Science)
10:10		Exploring proton mobility in the catalytic layer of High Temperature Fuel Cells
10:30	Coffee Break	
	Water and aquation	c solutions I
		Marie-Louise Saboungi (University Pierre and Marie Curie )
10:50	Invited Talk	Relaxation in a prototype ionic liquid and its mixture with water
		Paula Malo de Molina (Materials Physics Center)
		Microscopic Insights from Coherent and Incoherent Neutron Scattering on the
11:20		Dynamics of Liquid Water and Amino-Acid Solutions
	Water and aquation	c solutions II
		Alberto Striolo (University College London)
11:40	Invited Talk	Transport Mechanisms in Confinement: Are Molecular Simulations Helpful?
		Souleymane Diallo (Oak Ridge National Laboratory)
12:10		Characteristic Features of Water Dynamics in Confined Geometries
		R. Gregor Weiß (Humboldt-Universität zu Berlin)
12:30		Anomalies of hydrophobic solvation extend into water dynamics
		Jose M. Borreguero (Oak Ridge National Laboratory)
		Fast Water Exchanges on Aqueous Ions and a Mineral Surface Resolved Using
12:50		Molecular Dynamics Validated by Quasi-Elastic Neutron Scattering
13:10	Lunch	
	Polymers and mer	mbranes
		Henrich Frielinahaus (Forschunaszentrum Jülich)
		Amphiphilic Polymers with a Continuous Philicity Profile in Bicontinuous
14:10		Microemulsions Studied by Quasielastic Neutron Scattering
		Fabrizia Foalia (Imperial College London)
		Neutron backscattering study of polyamide and water dynamics in reverse osmosis
14:30		(RO) membranes
		Daniela Russo (Institut Laue-Langevin )
		Investigation into the relaxation dynamics of polymer-protein conjugates reveals
14:50		surprising role of polymer solvation on inherent protein flexibility
1.100	Biosystem I	
		Tilo Sevdel (Institut Laue-Langevin)
15.10	Invited Talk	High-resolution spectroscopy of proteins in solution
13.10		Tatsuhito Matsuo (National Institutes for Quantum and Radiological Science and
		Technology)
		Picosecond dynamics of F-actin myosin subfragment-1 and their hydration water
15.40		studied by quasielastic neutron scattering
16:00	Coffee Break	
10.00		Ramanrosad Mukhonadhyay (Bhabha Atomic Research Centre)
16.20	Invited Talk	Dynamical Features in Self Assembled Molecular Aggregates
10.20		ludith Peters (Institut Laue-Langevin)
		Pressure adaptive strategies in prokaryotes studied by quasi-elastic neutron
16.50		scattering
10.30		Maksym Golub (Université Grenoble Alnes)
		Combined SANS-OENS studies of low-density linonrotein under high hydrostatic
17.10		nrassura
17.10		Reate-Annette Brüning (Rielefeld University)
17.20		Structure and dynamics of phospholinid vesicles around the main phase transition
17.50	End	Structure and dynamics of phospholipid vesicles around the main phase transition
17.50	LIIU	

18:30 - 20:30

Potsdam Tour

Thursday, 8 <sup>th</sup> September 2016		
08:00	Registration for WIN	S
		Postersession for WINS in the breaks
	Biosystem II	
		Andreas Stadler (Forschungszentrum Jülich)
09:00	Invited Talk	Internal Protein Dynamics Investigated with Quasielastic Neutron Scattering
		Tilo Seydel (Institut Laue-Langevin)
		Quasi-elastic and Inelastic Neutron Scattering: Revealing confined liquid dynamics in
09:30		dental cements
		Stéphane Longeville (Laboratoire Léon Brillouin)
		Diffusion of hemoglobin in concentrated solutions and in blood cells: a Physiological
09:50		implication
10:10	Closure	
10:30	Coffee Break	

WINS 2	016	
	New Sources	
		Ulrich Rücker (Forschungszentrum Jülich)
10:50	Invited Talk	The High-Brilliance Neutron Source Project HBS
		Kenneth Herwig (Oak Ridge National Laboratory)
		Prospects at the Oak Ridge National Laboratory Spallation Neutron Source Second
11:10		Target Station
		Nico Bernt (University of Technology Dresden)
11:30		The Training and Research Reactor AKR-2
		Tetsuya Yokoo (J-Parc)
11:50		Recent progress on the spectrometers in J-PARC
		Rasmus Toft-Petersen (Technical University of Denmark)
12:10		Status of the spectroscopy instrument suite at the ESS
		Russel Ewings (STFC Rutherford Appelton Laboratory)
12:30		Developments at the ISIS Pulsed Neutron and Muon Source
12:50	Lunch Break	
	New instruments	
		Paul Steffens (Institut Laue-Langevin)
13:50	Invited Talk	Performance of the cold Three-Axis Spectrometer Thales @ ILL
		Rasmus Toft-Petersen (Helmholtz-Zentrum Berlin)
14:10		MultiFLEXX: A new multiplexing back-end for the FLEXX cold triple axis spectrometer
		Shinichi Itoh (KEK Japan)
14:30		High Resolution Chopper Spectrometer HRC and Neutron Brillouin Scattering
		Russell Ewings (STFC Rutherford Appleton Laboratory)
14:50		Status of the MAPS time-of-flight spectrometer upgrade
		Margarita Russina (Helmholtz-Zentrum Berlin)
15:10		New NEAT - design concept and commissioning results

		Markus Appel (Friedrich-Alexander Universität Erlangen-Nürnberg )
		The Backscattering And Time-of-flight Spectrometer Option BATS for IN16B: Concept,
15:30		Design & Future Developments
		Nicolas R. de Souza (Australien Nuclear Science and Technology Organisation)
		Design and first results from EMU, the high-resolution backscattering spectrometer at
15:50		ANSTO
16:10	Coffee Break	
		Ingo Hoffmann (Institut Laue-Langevin)
16:30	Invited Talk	The IN15 Upgrade
		Tatsuro Oda (Kyoto University)
		Experimental study on TOF-MIEZE type neutron spin echo spectroscopy at BL06 at J-
16:50		PARC/MLF
	Data collection	and instrument simulations
		Yukinobu Kawakita (J-Parc Center)
		Challenge on data analysis for inelastic and quasielastic neutron scattering for
17:10	Invited Talk	functional materials with structural disorder in real space and time
		Emmanuel Farhi (Institut Laue-Langevin)
17:30		Integrated simulation infrastructure for experiment planning: phonons
		Mads Bertelsen (University of Copenhagen)
17:50		McStas component for simulating multiple scattering in sample environment
18:10	End	
20:00 - 23	:00	Dinner (Boat trip) (Shuttle departs 19:00 in front of the Kutschstall)

Friday, 9 <sup>t</sup>	<sup>h</sup> September 2016	
10:00 - 12	:00	Guided Tour around the neutron guide hall
12:00	Lunch Break	
	Instrument compo	onents and new concepts
		Péter Harmat (ANTE Innovative Technologies)
		Turn-key large area modular detector system with event recording time-of-flight data
13:00	Invited Talk	acquisition for spectrometer NEAT: concept, design, performance
		Eugene Mamontov (Oak Ridge National Laboratory)
13:20		WAVES concept and steps toward its practical implementation at the SNS
		Felix Groitl (École Polytechnique Fédérale de Lausanne )
13:40		CAMEA — A novel multiplexing analyzer for neutron spectroscopy
		Stéphane Longeville (Technical University of Munich)
14:00		C-SPEC- a cold time of flight spectrometer for the ESS
		Nicolo Violini (JCNS)
14:20		T-REX: a bispectral chopper spectrometer for the ESS
		Antonio Benedetto (Paul Scherrer Institute )
14:40		An Instrument-Concept for Dynamics of Complex (Bio-) System from Elastic Scattering
		Feri Mezei (University of Messina )
		Correlation spectrometer for filtering of (quasi)elastic neutron scattering with
15:00		variable resolution
		Ramil Gainov (Helmholtz-Zentrum Berlin )
15:20		Concept of hybrid polarizing guide compressor for neutron spectrometers
15:40	Closure	
16:20	End of QENS/WINS	