Program

Sunday, 26th October, 2014

17:00 – 20:00	Registration
From 18:30	*BUFFET DINNER* / Informal get together

Monday, 27th October, 2014

07:30	*BREAKFAST*	
08:30 – 08:45	Martina Havenith Dominik Marx Wolfram Sander	**Welcome and opening**
08:45 – 09:00	Ernst Dreisigacker	**About the Wilhelm and Else Heraeus Foundation**
09:00 – 10:00	Christopher Hunter	**Molecular recognition probes of solvation phenomena**
10:00 – 10:45	R. Benny Gerber	**Solvation and chemical reactions of molecules on ices and in organic aerosols**
10:45 – 11:15	*COFFEE BREAK*	
11:15– 12:00	Ralf Ludwig	**Ion pairing in protic ionic liquids: The effects of solvent polarity, solvent concentration and temperature**
12:00 – 12:45	Othmar Steinhauser	**Computational solvation dynamics: Electric and magnetic probes**
12:45 – 12:50	**Conference Photo** (in front of the Physikzentrum)	
12:50	*LUNCH*	

Program

Monday, 27th October, 2014

14:30 – 15:15	Yunjie Xu	**Solvation of Chiral Molecules: VCD Signatures and Gas Phase Solvated Clusters**
15:15 – 15:30	Mychel Varner	**Role of solvation in the photoinitiated oxidation of ammonia**
15:30 – 15:45	Greg Dunning	**The onset of hydrogen bonding and subsequent solvent reorganisation following F-atom reactions in solution**
15:45 – 16:00	Janne Savolainen	**Two-dimensional Raman-terahertz spectroscopy of water**
16:00 – 16:30	*COFFEE BREAK*	
16:30 – 16:45	Ruth Livingstone	**Interfacial water dynamics – modified by the presence of a surfactant**
16:45 – 17:00	Johannes Hunger	**Heterogeneous dynamics in protic ionic liquids**
17:00 – 17:15	Daniel Muñoz	**Methanol oxidation at the TiO_2/H_2O interface in gas and liquid phases**
17:15 – 17:30	Ana Vila Verde	**Solvent-shared pairs of densely charged anions and cations supra-additively slowdown water rotation**
17:30 – 17:45	Alexander Schlaich	**Hydration interaction of polar surfaces**
17:45 – 18:00	Jozef Lengyel	**Photodissociation dynamics of hydrogen halides on ice nanoparticles**
18:00	*DINNER*	
19:30	**Postersession**	

Program

Tuesday, 28th October, 2014

07:30	*BREAKFAST*	
08:30 – 09:30	Eckhard Spohr	**Modelling interfacial electrochemistry with atomistic simulations. State of the art and challenges**
09:30 – 10:15	Maxim Fedorov	**Interfacial structural transitions in ionic liquids at charged surfaces: Recent insights from computer simulations**
10:15 – 10:45	*COFFEE BREAK*	
10:45 – 11:30	Jan-Dierk Grunwaldt	**In situ studies during heterogeneously catalysed oxidation reactions: From gas to liquid phase and supercritical fluids**
11:30 – 12:15	Osamu Sugino	**Electrochemical solid-liquid interface from first-principles**
12:15	*LUNCH*	
14:00	**Excursion** **Walking Tour and Wine Tasting**	
19:30	*HERAEUS DINNER* *(cold & warm buffet, free beverages)*	

Program

Wednesday, 29th October, 2014

07:30	*BREAKFAST*	
09:00 – 10:00	A. Joshua Wand	**Characterization of protein hydration by NMR**
10:00 – 10:45	Huib Bakker	**Structure of water at oil and protein surfaces studied with surface sum-frequency generation**
10:45 – 11:15	*COFFEE BREAK*	
11:15 – 12:00	Dor Ben-Amotz	**The emergence of structure from randomness in aqueous aggregation processes**
12:00 – 12:45	Jochen Blumberger	**Redox properties of solvated ions and proteins from density functional theory based and QM/MM molecular dynamics simulation**
12:45	*LUNCH*	
14:30 – 15:15	Nikolaus Ernsting	**Observing the hydration layer of trehalose with a linked molekular THz probe**
15:15 – 16:00	Ruth Gschwind	**Solvent effects in synthesis and catalysis insights by NMR**
16:00 – 16:30	*COFFEE BREAK*	

Program

Wednesday, 29th October, 2014

16:30 – 16:45	Hannah Gelman	**Protein stability *in vivo* and the intracellular environment**
16:45 – 17:00	Liel Sapir	**Theory of enthalpic depletion forces in complex solutions**
17:00 – 17:15	Matthias Heyden	**Resolving anisotropic distributions of correlated vibrational motion in protein hydration water**
17:15 – 17:30	Moran Grossmann	**Enzymatic turnover of macromolecules generates long lasting protein-water coupled motions beyond reaction steady-state**
17:30 – 17:45	Georgios Gerogiokas	**Biomolecular hydration thermodynamics via grid cell theory aids prediction of ligand-protein binding affinities**
17:45 – 18:00	Michael Senske	**Protein stabilization by macromolecular crowding through enthalpy rather than entropy**
18:00 – 18:15	Emiliano Brini	**Computing solvent-induced forces in the solvation approach called Semi Explicit Assembly**
18:15	*DINNER*	
19:45	**Postersession**	

Program

Thursday, 30th October, 2014

07:30	*BREAKFAST*	
09:00 – 09:45	Thomas Kiefhaber	**Fast conformational fluctuations in proteins and peptides measured by triplet-triplet energy transfer (TTET)**
09:45 – 10:30	Benjamin Schuler	**Probing the structure and dynamics of unfolded and intrinsically disordered proteins with single-molecule spectroscopy**
10:30 – 11:00	*COFFEE BREAK*	
11:00 – 11:45	Peter Vöhringer	**Ultrafast solvated electron dynamics in liquids and supercritical fluids**
11:45	**Poster Prize, Closing and Lunch**	

End of the seminar and departure