

Stockholm Discussion Meeting

Structure and Molecular Scale Properties of Liquid Water

Organized by Anders Nilsson and Lars G.M. Pettersson
 Location: AlbaNova University Center, Stockholm, Sweden
 June 14-16, 2006

PROGRAM

Tuesday June 13

Check in at Hotel Oden (<http://www.hoteloden.se/>)
 Evening reception

Wednesday June 14

08:30-12:45 Morning session

Moderator:	<i>Ivar Olovsson</i>	
08:30-08:45	Opening	
08:45-09:15	Thomas Elsässer	Ultrafast dynamics of intra- and inter-molecular vibrations in liquid H ₂ O
09:15-09:45	James Skinner	Dynamics, hydrogen bonding, and vibrational spectroscopy in liquid water
09:45-10:15	Dana Dlott	Ultrafast IR-Raman measurements of water vibrations
10:15-10:45	<i>Coffee</i>	
10:45-11:15	Rodolphe Vuilleumier	Infrared spectroscopy and atomic dynamical partial charges in liquid water
11:15-11:45	Kersti Hermansson	OH vibrations as a probe of the local environment in water
11:45-12:45	<i>Discussion</i>	
12:45-13:30	<i>Lunch</i>	

13:30-17:30 Afternoon session

Moderator:	<i>Börje Johansson</i>	
13:30-14:00	Anders Nilsson	X-ray Absorption Spectroscopy and X-ray Raman Scattering studies of liquid water
14:00-14:30	Giulia Galli	Structural and spectroscopic properties of water at ambient conditions and under confinement, from ab-initio calculations
14:30-15:00	Huib Bakker	Ultrafast dynamics of water in strong confinement
15:00-15:30	<i>Coffee</i>	
15:30-16:00	Lars Pettersson	Theoretical X-ray studies of liquid water
16:00-16:30	Mikko Hakala	X-ray Compton scattering as a probe of hydrogen bonds and local coordination in water
16:30-17:30	<i>Discussion</i>	
Evening	<i>Dinner</i>	

Thursday June 15
08:30-12:30 Morning session

Moderator:	<i>Sven Lidin</i>	
08:30-09:00	Uwe Bergmann	O-O RDF from EXAFS in Raman mode
09:00-09:30	Chris Benmore	Structural isotopic quantum effects in liquid water
09:30-10:00	Sean Brennan	Structural studies of liquid water using X-ray scattering
10:00-10:30	<i>Coffee</i>	
10:30-11:00	Teresa Head-Gordon	A Molecular View of Liquid Water from Theory and Experiment
11:00-11:30	Alan Soper	Joint structure refinement of neutron and X-ray data for water
11:30-12:30	<i>Discussion</i>	
12:30-13:30	<i>Lunch</i>	

13:30-17:30 Afternoon session

Moderator:	<i>Bengt Lundqvist</i>	
13:30-14:00	Roberto Car	Hydrogen bonds and intermolecular correlations in water
14:00-14:30	Glenn Martyna	Simulation studies of liquid water and peptide fragments in water by ab initio and empirical force field models: Investigating the role of model physics in structure determination.
14:30-15:00	Sotiris Xantheas	Local hydrogen bonding environment in liquid water
15:00-15:30	<i>Coffee</i>	
15:30-16:00	Fei Ling Zhang	TBA
16:00-16:30	Frank Weinhold	How the experimental water microstructure was theoretically predicted, how it makes sense, and why it is important
16:30-17:30	<i>Discussion</i>	
19:30-	<i>Buffet dinner</i>	Official reception and guided tour of the Stockholm City Hall http://www2.stockholm.se/cityhall/eng_tittain.htm#

The meeting is sponsored by the Henrik Granholm Foundation, the Royal Academy of Sciences through its Nobel Institute for Chemistry and by the Swedish Research Council

Friday June 16

08:30-12:30 Morning session

Moderator:	<i>Mats Larsson</i>	
08:30-09:00	Hajime Tanaka	Two-order-parameter model of water: Thermodynamic anomaly, the glass transition, and the liquid-liquid transition
09:00-09:30	Bernd Winter	Spectral finger print of liquid water in photoemission
09:30-10:00	Dennis Nordlund	Auger and photo-electron spectroscopy on liquid water
10:00-10:30	<i>Coffee</i>	
10:30-11:00	Clemens Heske Michael Zharnikov	X-ray emission spectroscopy of liquid water
11:00-11:30	Shik Shin	High resolution soft X-ray emission study on water
11:30-12:30	<i>Discussion</i>	
12:30-13:30	<i>Lunch</i>	

13:30-17:00 Afternoon session

Moderator:	<i>Bengt Kasemo</i>	
13:30-14:00	Alfred Laubereau	Ultrafast superheating and melting of ice
14:00-14:30	John Tse	XAS of ordered and amorphous ices - an experimental and theoretical study
14:30-15:00	Roger Klein	Modelling Liquid Water: Experimental ^{17}O -NMR, Electron Density Topology, NBO Analysis and $^1\text{H}/^{17}\text{O}$ Chemical Shielding Tensors Reflect Hydrogen Bond Structure, Coordination and Cooperativity
15:00-15:30	<i>Coffee</i>	
15:30-17:00	<i>Discussion</i>	Concluding discussion, summary and wrap-up

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