

MEETING AGENDA

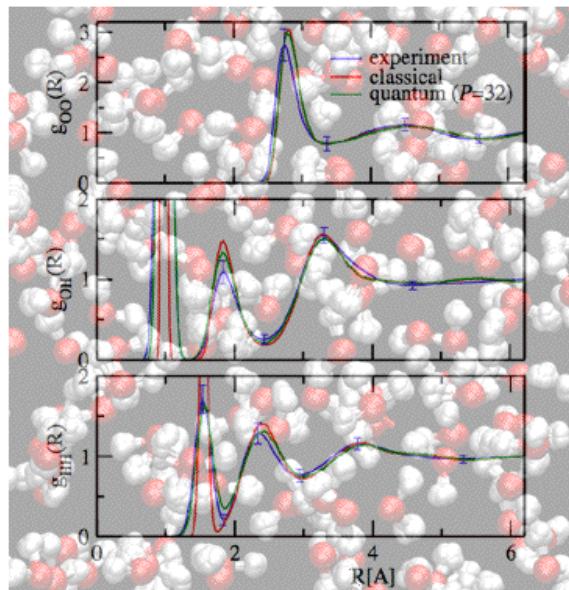
Aqueous Solutions And Their Interfaces

June 23rd – June 27th, 2008

Hotel Fodele Beach
Heraklion, Crete
GREECE

Ἄριστον μὲν ὕδωρ

Πίνδαρος, Ὀλυμπιακῆς Ὡδῆς 1, Στροφή 1, 476 π.Χ.



Water is the finest of all

PINDAR, Olympian Odes, Strophe 1, 476 B.C.

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***The Office of Naval Research,
The Center for Biophysical Modeling and Simulation – University of Utah
The University of Crete
Administrative Office, Region of Crete***

Sunday, June 22nd, 2008

Afternoon	<i>Arrival & Check-in</i>
17:00 – 18:00	<i>Registration</i>
18:00 – 21:00	<i>Welcome Reception / Dinner</i>

Monday, June 23rd, 2008

Morning Session

Session Chair: Theofanis N. Kitsopoulos – University of Crete

- 8:00 – 8:15** **General Remarks / Information / Logistics** (incl. accompanying persons)
Greg Voth / Sotiris Xantheas
- 8:15 – 8:30** **Welcome Address**
Theofanis Kitsopoulos – University of Crete
- 8:30 – 9:15** **The pH Of The Liquid Water Surface: Selective Adsorption Of Hydroxide And Hydronium**
Richard Saykally – University of California, Berkeley
- 9:15 – 10:00** **Second Harmonic And Sum Frequency Studies Of Equilibrium And Time Dependent Processes At Aqueous Interfaces**
Ken Eisenthal – Columbia University
- 10:00 – 10:15** **Coffee Break**
- 10:15 – 11:00** **Vibrational Spectroscopy Of Water Interfaces**
Ron Shen – University of California, Berkeley
- 11:00 – 11:45** **Water At Hydrophobic Surfaces: Insights Gained From A Combined Experimental And Theoretical Approach**
Geraldine Richmond – University of Oregon
- 11:45 – 12:30** **Why Ducks Don't Need A Towel: Dynamics Of Water Around Hydrophobes**
Huib Bakker – FOM Institute for Atomic and Molecular Physics
- 12:30 – 13:30** **Lunch Break**
- 13:30 – 16:00** **Free Time**

Afternoon / Evening Session

Session Chair: Francesco Paesani – University of Utah

- 16:00 – 16:45** **Ab Initio Quantum Mechanical Charge Field Molecular Dynamics: A Non-Parametrised First-Principle Approach To Liquid Systems Including Composite Solutes**
Bernd Rode – University of Innsbruck
- 16:45 – 17:30** **Electric Field Fluctuations At The Air-Water Interface**
Phillip Geissler – University of California, Berkeley
- 17:30 – 18:15** **Influence Of Concentration And Anion Size On The Hydration Of H⁺ Ions And Water Structure**
Maria Antonietta Ricci – University of Roma III
- 18:30 – 21:00** **Dinner**

Tuesday, June 24th, 2008

Morning Session

Session Chair: Sotiris S. Xantheas – Pacific Northwest National Laboratory

- 8:15 – 9:00** **Quantum Effects On The Structure Of Water**
Alan Soper – Rutherford Appleton Laboratory
- 9:00 – 9:45** **New Experimental X-Ray Studies Of Bulk Water; Indications Of Spatially Separated Two Structural Motifs**
Anders Nilsson – Stanford University
- 9:45 – 10:30** **Theoretical And Experimental Investigations Of Bulk Water And Water At Biological Interfaces**
Teresa Head-Gordon – University of California, Berkeley
- 10:30 – 10:45** **Coffee Break**
- 10:45 – 11:30** **Ultrafast Bulk And Interfacial Melting Of Ice, Investigated By Time-Resolved Infrared Spectroscopy**
Alfred Laubereau – Technical University of Munich at Garching
- 11:30 – 12:15** **Theoretical Simulation Of X-Ray And Vibrational Spectroscopy Data On Bulk Liquid Water**
Lars G. M. Pettersson – University of Stockholm
- 12:15 – 13:00** **Is Nuclear Quantization Important To Understand The Behavior Of Water?**
Francesco Paesani – University of Utah
- 13:00 – 13:45** **Lunch**
- 13:45 – 14:30** **Free Time**
- 14:45** **Bus Leaves Hotel**
- 15:00 – 18:00** **Visit Of The Archaeological Site Of Knossos**
- 18:30 – 21:00** **Dinner**

Wednesday, June 25th, 2008

Morning Session

Session Chair: James L. Skinner – University of Wisconsin

- 8:15 – 9:00** **Time-Resolved Dynamics Of Charge-Transfer-To-Solvent States In Anion Clusters**
Dan Neumark – University of California, Berkeley
- 9:00 – 9:45** **Accommodation Of Excess Electrons And Protons By Water Clusters**
Ken Jordan – University of Pittsburgh
- 9:45 – 10:00** **Composite And Asymmetrically Solvated Ions In Solution**
Thomas Hofer – University of Innsbruck
- 10:00 – 10:15** **Coffee Break**
- 10:15 – 11:00** **Pump-Probe Studies Of Isomer Interconversion In H-Bonded Clusters**
Mark Johnson – Yale University
- 11:00 – 11:45** **Solvation And Reactivity Of OH Radicals In Aqueous Systems**
Bruce Garrett – Pacific Northwest National Laboratory
- 11:45 – 12:30** **The Excess Proton In Water: Past Predictions And New Discoveries**
Greg Voth – University of Utah
- 12:30 – 13:30** **Lunch Break**
- 13:30 – 16:00** **Free Time**

Afternoon / Evening Session

Session Chair: Thomas S. Hofer – University of Innsbruck

- 16:00 – 16:45** **Vibrational Spectroscopy And Hydrogen Bonding In Bulk Water, At The Liquid/Vapor Interface, And In Salt Solutions**
Jim Skinner – University of Wisconsin
- 16:45 – 17:30** **Structure And Dynamics Of Water At The Interface Of Phospholipid Membranes**
Roberto Righini – University of Florence
- 17:30 – 17:45** **Solution Structure Of NaNO₃ In Water: Diffraction And Molecular Dynamics Simulation Study**
Szabolcs Bálint – Hungarian Academy of Sciences
- 18:30** **Bus Leaves Hotel**
- 19:00 – 22:30** **Conference Banquet At “Boutaris” Winery**

Thursday, June 26th, 2008

Morning Session

Session Chair: Gregory A. Voth – University of Utah

- 8:15 – 9:00** **Computer Simulation Studies Of Water/Hydrocarbon And Water/Surfactant Interfaces**
Branka Ladanyi – Colorado State University
- 9:00 – 9:45** **Water In Nonpolar Pores And Protein Cavities**
Gerhard Hummer – National Institutes of Health
- 9:45 – 10:00** **Molecular Dynamics Study Of Water Adsorbed On Mixed Self-Assembled Monolayers As Proxies For Atmospheric Organic Surfaces**
Martina Roeselová – Academy of Sciences of the Czech Republic
- 10:00 – 10:15** **Coffee Break**
- 10:15 – 11:00** **Liquid And Glassy Water In Nano-Scale Confinement**
Pablo Debenedetti – Princeton University
- 11:00 – 11:45** **Nanophase Segregation In Super-Cooled Aqueous Solutions Driven By Water Polyamorphism**
Valeria Molinero – University of Utah
- 11:45 – 12:30** **Models For Describing The Interactions Between Water Molecules**
Sotiris Xantheas – Pacific Northwest National Laboratory
- 12:30 – 13:30** **Lunch Break**
- 13:30 – 16:00** **Free Time**

Afternoon / Evening Session

Session Chair: Martina Roeselová – Academy of Sciences of the Czech Republic

- 16:00 – 16:45** **Peculiar Structural And Dynamic Properties Of Interfacial Water**
Marie-Claire Bellissent-Funel – LLB (CEA-CNRS), Saclay
- 16:45 – 17:30** **Trapping Proton Transfer Intermediates In The Disordered H-Bonded Network Of Cryogenic Hydrofluoric Acid Solutions**
Patrick Ayotte – Sherbrooke University
- 17:30 – 17:45** **The Nature Of Contact Ion-Pair Acid Dissociation Intermediates In Water: A Computational Infrared Spectroscopy Approach**
Radu Iftimie – University of Montreal
- 19:00 – 22:00** **Greek Night At “Elia” Restaurant (Fodele Beach Hotel)**

Friday, June 27th, 2008

Morning Session

Session Chair: Richard J. Saykally – University of California, Berkeley

- 8:00 – 8:45** **Balancing Local Order And Long-Ranged Interactions In The Molecular Theory Of Liquid Water And Its Interfaces**
Lawrence Pratt – Tulane University
- 8:45 – 9:30** **Specific Ion Effects At Air-Water And Surfactant-Water Interfaces**
Doug Tobias – University of California, Irvine
- 9:30 – 10:15** **Hydrophobic To Hydrophilic Hydration Of Solutes And Interfaces**
Shekhar Garde – Rensselaer Polytechnic Institute
- 10:15 – 10:30** **Coffee Break**
- 10:30 – 11:15** **Analyzing Intermolecular Interactions From Electronic Structure Calculations And The Nature Of The Water-Water Hydrogen Bond**
Martin Head-Gordon – University of California, Berkeley
- 11:15 – 12:00** **Ab-Intio Simulations Of Water In Contact With Non-Polar Surfaces**
Giulia Galli – University of California, Davis
- 12:00 – 12:30** **Concluding Remarks**
- 12:30 – 13:30** **Lunch Break**
- 14:00** **Departure**

Saturday, June 28th, 2008

Optional 1-day trip to Santorini