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Structure and Dynamics of Water and Aqueous Solutions

6-8 December 2010

PCTS – Jadwin Hall
Fourth Floor, Room 407

Organizers
Roberto Car, Giulia Galli, John Rehr

Co-sponsored by Computational Materials and Chemical Sciences Network

Structure and Dynamics of Water and Aqueous Solutions

Monday, 6 December 2010

7:45 - 8:55 Registration and Breakfast at PCTS

8:55 - 9:10 Opening (welcome address + introduction to CMCS network)

Morning session: C*hair, Giulia Galli*

9:10 - 9:50 Ab-initio liquid water: present and future challenges
Roberto Car, Princeton University

9:50 - 10:30 LIQUID WATER, THE MOST "COMPLEX" LIQUID AND SOLVENT: New Spectroscopic Results in Nanoconfined and Biological Environments and Their Possible Interpretation
Eugene Stanley, Boston University

10:30 Coffee break

11:00 - 11:25 The structure of ambient water.
Teresa Head Gordon, UC Berkeley & Lawrence Berkeley National Laboratory

11:25 - 11:50 Isotopic quantum effects and the 1st peak in the O-O pair distribution function in water.
Christopher Benmore, Argonne National Laboratory

11:50 – 12:15 Structural changes in compressed water.
Eric Schwegler, Lawrence Livermore National Laboratory

12:15 - 2:00 Lunch break

Afternoon session: C*hair, Roberto Car*

2:00 - 2:40 X-Ray Spectroscopy and Scattering Studies of Water.
Anders Nilsson, Stanford University

2:40 – 3:05 XAS and XES simulations using transition-potential and semi-classical Kramers-Heisenberg techniques.
Lars Pettersson, Stockholm University

3:05 - 3:30 Aqueous solvation explored using x-ray spectroscopy.
David Prendergast, Lawrence Berkeley National Laboratory

3:30 Coffee break

Structure and Dynamics of Water and Aqueous Solutions

Monday, 6 December 2010- Continued

4:00 – 4:25 Many-Body Techniques in Calculations of Optical and X-Ray spectra
John Rehr, University of Washington

4:25 - 4:50 GW/BSE Calculations of Optical and X-Ray Spectra of Liquid and Solid H_2O.
John Vinson, University of Washington

4:50 – 5:15 QM/MM meets Many-Body Perturbation Theory: application to indole in water solution
Adriano Mosca Conte, University of Rome

5:15 - 5:40 X-Ray Absorption Signatures of the Molecular Environment in Water and Ice
Xifan Wu, Temple University

Tuesday, 7 December 2010

8:00 - 9:00 Breakfast at PCTS

Morning session: C*hair, John Rehr*

9:00 - 9:40 Hydration phenomena at the nanoscale
Pablo Debenedetti, Princeton University

9:40 - 10:05 Confined water: first principle calculations
Giulia Galli, UC Davis

10:05 - 10:30 Molecular simulations of water-silica interactions and nanoconfined water
Steve Garofalini, Rutgers University

10:30 Coffee break

11:00 - 11:25 Explicit solvation in ab-initio simulations and optical properties of water
Jerzy Bernholc, North Carolina State University

11:25 – 11:50 Dispersion effects in liquid water
Omolulu Akin-Ojo, International Centre for Theoretical Physics

11:50 - 12:15 Van der Waals forces resolve controversy on water structure, providing room for high density fluctuations
Andreas Moegelboej, Technical University of Denmark

Structure and Dynamics of Water and Aqueous Solutions

Tuesday, 7 December 2010- Continued

12:15 – 2:00 Lunch break

Afternoon session: C*hair, Michele Parrinello*

2:00 – 2:40 Computational Research on Water at PNNL: Issues and Approaches
Bruce Garrett, Pacific Northwest National Laboratory

2:40 - 3:05 Structure and dynamics of OH-(aq) from ab initio molecular dynamics
Mark Tuckerman, New York University

3:05 - 3:30 First-principle simulations of the infra red spectrum of liquid water using hybrid density functional theory
Cui Zhang, University of California, Davis

3:30 Coffee break

4:00 - 4:25 Zero point kinetic energy and quantum effects on the proton momentum distribution in water
Roberto Senesi, University of Rome

4:25 - 4:50 Nuclear quantum effects and the potential energy surface in hexagonal ice
Lin Lin, Princeton University

4:50 - 5:15 Coloring path integrals: an accelerated method to model nuclear quantum effects
Michele Ceriotti, ETHZ, Switzerland

Structure and Dynamics of Water and Aqueous Solutions

Wednesday, 8 December 2010

8:00 - 9:00 Breakfast at PCTS

9:00 – 10:30 Organized round table discussion

10:30 Coffee break

11:00 – 12:15 Organized round table discussion

12:15 – 2:00 Lunch