The Abdus Salam International Centre for Theoretical Physics

Structure and Dynamics of Hydrogen-Bonded Systems

Cosponsor(s): co-sponsored by: Centre for Molecular Structure and Dynamics, STFC, UK
Organizer(s): Directors: J. Kohanoff, S. Koval, R. Senesi Local Organizer: E. Tosatti
Trieste - Italy, 26 - 27 October 2009

Venue: Leonardo da Vinci Building Main Lecture Hall

Final programme

MONDAY, 26 OCTOBER 2009 (Room:Leonardo da Vinci Building Main Lecture Hall)

26 October 2009

08:30 - 09:00 (Room: Leonardo da Vinci Building, Lobby)
--- REGISTRATION & ADMINISTRATIVE FORMALITIES ---

09:00 - 09:05 **OPENING SESSION**

Session 1 - ICE AND ITS SURFACE (in honor of Victoria Buch) (Room:Leonardo da Vinci Building Main Lecture Hall)

26 October 2009

09:00 - 09:25 **Erio TOSATTI** / *SISSA, ICTP & CNR/INFM Democritos, Trieste, Italy*
Ice and Victoria Buch: a cold surface and a warm heart

09:25 - 09:50 **Thomas KUEHNE** / *Harvard University, Cambridge, U.S.A.*
The aqueous liquid-vapor interface: new insights from a novel Car-Parrinello-like approach to Born-Oppenheimer molecular dynamics

09:50 - 10:15 **Olivia PULCI** / *Universita' di Roma II "Tor Vergata", Italy*
Effect of proton disorder in the excited state properties of ice

10:15 - 10:40 **Livia BOVE** / *Universite' Pierre et Marie Curie Paris VI, Paris, France*
Concerted proton tunnelling in ordinary ice

10:40 - 11:10 (Room: Leonardo da Vinci Building, Lobby)
--- COFFEE BREAK ---

SESSION 2 - LIQUIDS (Room:Leonardo da Vinci Building Main Lecture Hall)

26 October 2009

11:10 - 11:50 **Alan SOPER** / *Rutherford Appleton Laboratory, Didcot, U.K.*
Is ambient water homogeneous or inhomogeneous?

11:50 - 12:30 **Tristan YOUNGS** / *The Queen's University of Belfast, U.K.*
Molecular solvents over heterogeneous surfaces and ionic liquids in the bulk - experimental and theoretical study of hydrogen bonding systems

12:30 - 14:00 (Room: Leonardo da Vinci Building Cafeteria)
--- LUNCH BREAK ---

14:00 - 14:40 **Carla ANDREANI** / *Universita' di Roma II "Tor Vergata", Italy*
Proton quantum effects in water

14:40 - 15:20 **Joseph MORRONE** / *Columbia University, New York, U.S.A.*
Nuclear quantum effects in water: a study in position and momentum space

15:20 - 16:00 **David MANOLOPOULOS** / *University of Oxford, U.K.*
Competing quantum effects in liquid water

16:00 - 16:30 (Room: Leonardo da Vinci Building, Lobby)
--- COFFEE BREAK ---

16:30 - 17:10 **Ruth LYNDEN-BELL** / *University of Cambridge, U.K.*
Simulations of water and artificial liquids with weakened hydrogen bonds

17:10 - 17:50 **Chick WILSON** / *University of Glasgow, U.K.*
The evolution of hydrogen bonds in molecular materials under changing external conditions by neutron diffraction and complementary methods

17:50 - 18:30 --- BREAK & REFRESHMENTS ---

18:30 - 20:00 **POSTER SESSION**
Poster Gallery (behind the Main Lecture Hall)

20:00 - 23:00 --- SOCIAL DINNER ---

TUESDAY, 27 OCTOBER 2008 (Room:Leonardo da Vinci Building Main Lecture Hall)

27 October 2009

08:30 - 09:00 (Room: Leonardo da Vinci Building, Lobby)
--- REGISTRATION & ADMINISTRATIVE FORMALITIES ---

SESSION 3 - SOLIDS (Room:Leonardo da Vinci Building Main Lecture Hall)

27 October 2009

09:00 - 09:30 **Biswajit SANTRA** / *FHI der Max-Planck-Gesellschaft, Berlin, Germany*
On the accuracy of density-functional theory exchange-correlation functionals for hydrogen bonds in water

09:30 - 09:50 **Jorge KOHANOFF** / *The Queen's University of Belfast, U.K.*
Quantization of vibrations in H-bonded crystals

09:50 - 10:20 **Keith REFSON** / *Rutherford Appleton Laboratory, Didcot, U.K.*
Strong anharmonicity and isotope effects in Cr00H/Cr00D

10:20 - 10:40 **Sergio KOVAL** / *Universidad Nacional de Rosario, Argentina*
H-bonded Ferroelectrics from first-principles and derived modeling

10:40 - 11:00 (Room: Leonardo da Vinci Building, Lobby)
--- COFFEE BREAK ---

11:00 - 11:30 **John LOVEDAY** / *University of Edinburgh, U.K.*
High pressure structural studies of hydrogen bond centring

11:30 - 12:00 **Mark JOHNSON** / *Institut Max Von Laue-Paul Langevin, Grenoble, France*
Proton dynamics in short hydrogen bonds: two-site hopping in a single-well potential

SESSION 4 - LIQUID/SOLID INTERFACES (Room:Leonardo da Vinci Building Main Lecture Hall)

27 October 2009

12:00 - 12:30 **Pepa CABRERA-SANFELIX** / *Donostia International Physics Center, San Sebastian, Spain*
Water adsorption on 0/Ru(0001): Dissociation and cooperative effects

12:30 - 13:00 **Angelos MICHAELIDES** / *University College London, U.K.*
The quantum nature of the proton in water-hydroxyl overlayers on metal surfaces

13:00 - 14:00 (Room: Leonardo da Vinci Building Cafeteria)
--- LUNCH BREAK ---

SESSION 5 - CHEMISTRY/BIOLOGICAL SYSTEMS (Room:Leonardo da Vinci Building Main Lecture Hall)

27 October 2009

14:00 - 14:40 **Martina HAVENITH** / *Ruhr-Universitaet Bochum, Germany*
Chemistry below 1 K: Observation of the smallest droplet of acid

14:40 - 15:10 **Mariana ROSSI** / *FHI der Max-Planck-Gesellschaft, Berlin, Germany*
Secondary structure of H-bonded Polyalanine peptides in vacuo: Computational spectroscopy and DFT

15:10 - 15:50 **Raul CACHAU** / *National Cancer Instiute, Frederick, U.S.A.*
Study of mobile protons in enzymes as revealed by subatomic x-ray and neutron diffraction experiments

15:50 - 16:20 (Room: Leonardo da Vinci Building, Lobby)
--- COFFEE BREAK ---

16:20 - 17:00 **Janez MAVRI** / *National Institute of Chemistry, Ljubljana, Slovenia*
Dynamics of proton transfer in biological systems

17:00 - 17:20 **Roberto SENESI** / *II Universita' di Roma "Tor Vergata", Italy*
Proton momentum distribution of water confined in nanopores, protein hydration shells and DNA

SESSION 6 - CONFINED SYSTEMS (Room:Leonardo da Vinci Building Main Lecture Hall)

27 October 2009

17:20 - 17:50 **Jonas BJOERK** / *University of Liverpool, U.K.*
Hydrogen-bonding in bi-component supramolecular nanoporous networks

17:50 - 18:10 **CLOSING SESSION**