



Structure and Dynamics of Hydrogen-Bonded Systems

26 - 27 October 2009

(Miramare - Trieste, Italy)

The Abdus Salam International Centre for Theoretical Physics (ICTP) is organizing a two day Meeting on the **Structure and Dynamics of Hydrogen-Bonded Systems** to be held at the ICTP, Trieste, Italy from **26 - 27 October 2009**.

DESCRIPTION: Hydrogen-bonding is ubiquitous in physical, chemical, and biological sciences. At the root of the unique properties of water and of polymorphism in ices and in organic crystals, it is also involved in most biochemical processes such as enzyme catalysis. Protons and deuterons in hydrogen bonds behave as quantum-mechanical particles and, as such, they give rise to a variety of interesting quantum phenomena such as tunneling and geometric effects. Recent advances in neutron and X-ray scattering provide the tools for the accurate determination of the structure and dynamics of protons in hydrogen bonds. For example, deep inelastic neutron scattering recently showed, for the first time, direct evidence of proton tunneling in KDP. Parallel to that, advances in computational techniques such as path integral and wave function methods have allowed for the introduction of quantum nuclear effects on the theory of structural and dynamical properties of these systems. Classical and quantum molecular dynamics methodologies are frequently used as a complementary tool to the experimental ones. The coming together of all these elements makes this an extremely exciting time for the field, a time when substantial advances in our understanding of hydrogen bonded systems appear possible. The focus of this meeting will be on cutting-edge experimental and computational approaches, and on recent results aiming at describing and understanding the peculiarities of hydrogen-bonded systems in condensed phases such as solids, liquids, and macromolecular systems.

TOPICS:

- Structure and dynamics of hydrogen-bonded liquids and solids
- Hydrogen-bonded systems in confined geometries
- Biomolecular systems: proteins and DNA
- Polymorphism, High pressure phases and phase diagrams
- Water and aqueous solutions
- Ferroelectric ices
- Neutron Diffraction
- Compton and quasi-elastic neutron scattering
- X-ray diffraction and inelastic scattering
- Pump-probe spectroscopy
- Classical and Quantum Molecular Dynamics
- Ab initio electronic structure calculations
- Path integral methods
- Wave function methods for vibrations

PARTICIPATION: Scientists and students from all countries that are members of the United Nations, UNESCO or IAEA may attend. As the Meeting will be conducted in English, participants should have an adequate working knowledge of this language. Although, the main purpose of the Centre is to help research workers from developing countries, through a programme of training activities within a framework of international cooperation, a limited number of students and post-doctoral scientists from developed countries are also welcome to attend.

As a rule, travel and subsistence expenses of the participants should be borne by their home institution. Every effort should be made by candidates to secure support for their fare. However, very limited funds are available for partial support of some participants who are nationals of, and working in, a developing country, and who are not more than 45 years old. Such support is available only for those who attend the entire activity. **There is no registration fee for attending this Meeting.**

HOW TO APPLY FOR PARTICIPATION

The Application Form can be accessed at the activity website
<http://agenda.ictp.it/smr.php?2054>.

Once in the website, comprehensive instructions will guide you step-by-step, on how to fill out and submit the Application Form.

ACTIVITY SECRETARIAT:

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Co-sponsored by:

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ORGANIZERS:

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LOCAL ORGANIZER:

Erio TOSATTI
(ICTP-SISSA-Democritos, Trieste, Italy)

INVITED SPEAKERS:

Christiane Alba-Simionesco (Saclay, France)

Carla Andreani (Rome, Italy)

Huib Bakker * (Amsterdam, Netherlands)

Raul E. Cachau * (NIH, USA)

Roberto Car * (Princeton, USA)

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Ruth M. Lynden-Bell (Cambridge, UK)

David Manolopoulos (Oxford, UK)

Janez Mavri (Ljubljana, Slovenia)

Alan K. Soper (ISIS, UK)

Chick Wilson (Glasgow, UK)

Tristan Youngs (Belfast, UK)

* to be confirmed

**Deadline for
Requesting Participation:**

15 JUNE 2009