



**EAU AUX INTERFACES: NOUVEAUX DEVELOPPEMENTS EN PHYSIQUE, CHIMIE ET BIOLOGIE**

**WATER AT INTERFACES: NEW DEVELOPMENTS IN PHYSICS, CHEMISTRY AND BIOLOGY** (April 15-26, 2013)

*The programme of the School includes lectures (one hour and a half per lecture), as listed below, seminars (45 minutes or one hour per seminar), short talks and a poster session.*

- **Part 1: From Bulk to Nanoconfined Water** (Structure and dynamics, hydrogen-bonding, water-ice transformations)
  - (i) Spectroscopic probes: neutrons, X-rays, NMR, FTIR, Raman
  - (ii) Modelling

**M.-C. Maurel** (Paris): *Liquid water and the origins of life*

**J. Teixeira** (LLB, France): *Bulk and confined water*

**W. Kuhs** (Göttingen University, Germany): *Nanoscale atmospheric pressure ice*

**T. Loerting** (Innsbruck University, Austria): *Recent experimental developments in amorphous ices and their relation to deeply supercooled liquids*

**L. G. M. Pettersson** (Department of Physics, Stockholm University, S-106 91 Stockholm, Sweden): *Fluctuations in Ambient Water*

- **Part 2: Water /Solid Substrates**
  - (i) Interfacial interactions : hydrophobicity/hydrophilicity
  - (ii) Surface characterisation
    - Silicas (sol-gel, Vycor, CPG, MCM, SBA), Zeolites, clays
    - Activated carbons, carbon nanotubes.
  - (iii) Structure and dynamics (constrained molecular mobility), water-ice transformations
  - (iv) Spectroscopic probes: neutrons, X-rays, NMR, FTIR, Raman, fs-IR, THz-TDS

**A. Soper** (ISIS, UK): *The structure of water in bulk and in confinement by neutron and x-ray scattering*

**P. Varilly** (Cambridge, UK): *Fluctuations in water and their relation to the hydrophobic effect near model surfaces and proteins*

**T. Iiyama** (Shinshu University, Japan): *Structural Understanding of Water Confined in Hydrophobic Nanopores*

Other info in the organizer's guide at :  
<http://houches.ujf-grenoble.fr>

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**T. Yamaguchi** (Fukuoka, University, Japan): *Thermal behaviour, structure and dynamics of low-temperature water confined in mesoporous materials*

**M. Vogel** (Darmstadt, Germany): *NMR studies on rotational and translational motions of water in protein and silicate matrices*

- **Part 3: Water / Soft Substrates**

- (i) Related systems-clathrates, aqueous solutions, amphiphiles, surfactants, lamellar liquid crystals, microemulsions, soluble polymers, ionic liquids
- (ii) Structure and dynamics (constrained molecular mobility), hydrogen-bonding
- (iii) Spectroscopic probes: neutrons, X-rays, NMR, FTIR, Raman, fs-IR, THz-TDS

**J. Swenson** (Goteberg, Sweden): *The anomalous properties of water for the dynamics and the glass transition of proteins*

**A.S. Pensado** (Universität Leipzig, Germany): *Ionic liquids and water in touch: A theoretical study*

**Y. Ouchi** (Nagoya University, Japan): *Nonlinear Vibrational Spectroscopy and Molecular Dynamics Simulations on Water/Ionic Liquid Interfaces"*

**A. Deriù** (Parma University, Italy): *Structural and Dynamic Properties of Organised Structures of Saccharide Systems in Aqueous Solution*

**S. Meech** (University of East Anglia, Norwich, UK): *Time Domain Optical Kerr Effect Studies of Aqueous Solution: Ions to Proteins*

**T. Elsaesser** (Max-Born-Institut, Berlin, Germany): *Ultrafast dynamics in the hydration of phospholipid reverse micelles and DNA*

- **Part 4: Water / Biological Interfaces 1**

- (i) Biological interfaces, membranes, proteins, biological complexes, cells
- (ii) Interfacial water in biological processes, enzymatic catalysis, water channels, ionic channels
- (iii) Spectroscopic probes: neutrons, X-rays, NMR, FTIR, Raman, dielectric relaxation
- (iv) Molecular modelling, molecular dynamics, DFT computations, etc
- (v) Interaction potentials, simple and otherwise, ab initio methods
- (vi) Hydrogen-bond effects on structure and dynamics in confinement

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**F. Sterpone** (IBPC, Paris): *The protein hydration layer: how different from the bulk? A mirror for protein conformations and stability.*

**A. Oleinikova** (Darmstadt University, Germany): *Thermodynamic properties of hydration water: from model surfaces to the surfaces of biomolecules*

**M. Tarek** (France): *Simulation of hydrated membranes*

**J.-M. Zanotti** (LLB, France): *Evidences for coexisting distinct phases in interfacial water*

**M. Weik** (IBS, France): *Proteins need it wet. Don't they?*

• **Part 5: Water / Biological Interfaces 2**

- (i) Biological interfaces, membranes, proteins, biological complexes, cells
- (ii) Interfacial water in biological processes, enzymatic catalysis, water channels, ionic channels
- (iii) Spectroscopic probes: neutrons, X-rays, NMR, FTIR, Raman, dielectric relaxation
- (iv) Molecular modelling, molecular dynamics, DFT computations, etc
- (v) Interaction potentials, simple and otherwise, ab initio methods
- (vi) Hydrogen-bond effects on structure and dynamics in confinement

**G. Zaccai** (IBS, Grenoble): *Neutrons reveal the ecology of protein and water dynamics*

**B. Bouvier** (Lyon): *Water in biomolecular recognition processes - the forgotten partner*

**Halina Abramczyk** (Technical University of Lodz, Lodz, Poland): *Hydrogen bonds of interfacial water in human breast cancer tissue*

**P. Marquet** (Lausanne, Switzerland): *The water movements mediated by neuronal activity explored with digital holographic microscopy*