

ESI/CECAM Workshop on
“Water at Interfaces: From Proteins to Devices”
November 29 – December 2, 2016

organized by

**Valentino Bianco (U Vienna), Ivan Coluzza (U Vienna), Barbara Capone (U Vienna),
Christoph Dellago (ESI, U Vienna)**

• **Tuesday, November 29, 2016**

Session 1

14:00 – 14:40 *Registration*

14:40 – 15:25 **Rahul Raveendran Nair**

Molecules at two-dimensional interfaces and capillaries

15:25 – 16:10 **Sandrine Lyonnard**

Water Confined in Fuel Cell Membranes

16:10 – 16:40 *coffee / tea break*

16:40 – 17:25 **Laurent Joly**

Water friction on graphene and boron nitride surfaces: insight from ab initio molecular dynamics

17:25 – 18:10 **Maarten Biesheuvel**

Water desalination using Capacitive Electrodes: from Carbon Nanotube Membranes to Activated Carbon Suspensions – Concepts and Mean-field Transport Theory

• **Wednesday, November 30, 2016**

Session 2

09:00 – 09:45 **Huib Bakker**

Structure and dynamics of water molecules at protein surfaces

09:45 – 10:30 **Giancarlo Franzese**

A Multiscale Approach for Water at Bio-Nano Interfaces

10:30 – 11:00 *coffee / tea break / poster session*

11:00 – 11:45 **Valentino Bianco**

The role of water in the selection of stable proteins at ambient and extreme thermodynamic conditions

11:45 – 12:30 **Giorgio Schirò**

Unveiling the Role of Hydration Water in the Onset of Protein Structural Dynamics

12:30 – 15:00 *lunch break*

Session 3

15:00 – 15:45 **Biman Bagchi**

Protein Hydration Dynamics and Hydrophobic Force Law

15:45 – 16:30 **Xavier Barril**

The Quasi-Bound State of Protein-Ligand Complexes. Implications in Drug Discovery

16:30 – 17:00 *coffee / tea break / poster session*

17:00 – 17:45 **Max Paoli**

The Role of Science for Sustainable Development

19:30 *Social Dinner*

• **Thursday, December 1, 2016**

Session 4

09:00 – 09:45 **Sylvie Roke**

Snapshots of Ion Induced Long-range Structure in Aqueous Systems

09:45 – 10:30 **Francesco Mallamace**

An NMR study on the hydrophilic and hydrophobic interactions

10:30 – 11:00 *coffee / tea break / poster session*

11:00 – 11:45 **Simone Meloni**

The Salvinia Paradox: how the hydrophilic patches help keeping the plants surface dry

11:45 – 12:30 **Fabio Bruni**

The putative liquid-liquid transition is a liquid-solid transition in water confined in MCM

12:30 – 14:30 *lunch break*

Session 5

14:30 – 15:15 **Martin Chaplin**

Just how anomalous is interfacial water?

15:15 – 16:00 **Othmar Steinhauser**

Water Dynamics near biological surfaces studied by Shell-Resolved Computational Spectroscopy

16:00 – 16:30 *coffee / tea break / poster session*

16:30 – 17:15 **Martina Havenith**

THz spectroscopy and Solvation Science

17:15 – 18:00 **Ana Vila Verde**

Supra-additive slowdown of water rotation by outer-sphere ion pairs

• **Friday, December 2, 2016**

Session 6

09:00 – 09:45 **Hinrich Grothe**

Biological Ice Nucleation in the Atmosphere and the Biosphere

09:45 – 10:30 **Klaus Liedl**

Water Ordering at Protein Interfaces and Consequences for Biomolecular Recognition

10:30 – 11:00 *coffee / tea break*

11:00 – 11:45 **Eduardo Sanz**

The Role of the Ice-water Interface in Homogeneous Ice Nucleation

11:45 – 12:30 **Alexander Bittner**

Imaging thin water layers on single viruses

12:30 – 12:45 *Closing Word*

All talks take place at the ESI, Boltzmann Lecture Hall!