PROGRAM

Thursday - February 7, 2013

14:45-15:00 ***OPENING***

Session I: Chair J. Martí

15:00-15:20 **Fernando Bresme**
Computer simulation studies of heat conduction in water: bulk and interfaces

15:20-15:40 **Jordi Faraudo**
The missing link between the Hydration Force and interfacial water: Evidence from computer simulations

15:40-16:00 **Josep Bonet**
Dynamics of encapsulated water inside Mo132 cavities, and other aspects of confined water

16:00-16:20 **Juan José Saenz**
Capillary Adhesion Forces in Atomic Force Microscopy

16:20-16:40 **Giancarlo Franzese**
Water at biological and inorganic interfaces

16:40-17:00 **Claudio Cerdeiriña**
Compressible cell liquids for waterlike liquid-liquid criticality

17:00-17:40 ***COFFEE BREAK AND POSTER SESSION***

Session II: Chair G. Franzese

17:40-18:00 **Enrique Lomba**
Simple water-like models in one dimension

18:00-18:20 **Carlos Vega**
Describing water using computer simulation

18:20-18:40 **José Luis F. Abascal**
Propiedades del agua en condiciones extremas: región subenfriada y presiones negativas

18:40-19:00 **Chantal Valeriani**
Cavitation of water at negative pressure

19:00-19:20 **Eduardo Sanz**
The critical size of ice clusters in water freezing from simulations

21:30-23:00 ***DINNER***

Friday - February 8, 2013

Session III: Chair J. Faraudo

9:00-9:20 **Enrique Sanchez-Marcos**
Computer simulations of metal ions in aqueous solutions

9:20-9:40 **Diego González-Salgado**
Molecular simulation of the {methanol+water} system: structure and thermodynamics

9:40-10:00 **Felix Llovell**
Insights into the behavior of organic compounds in water

10:00-10:20 **Carles Calero**
Simulation and theoretical study of the H^1-NMR relaxation times in bulk water and aqueous ionic solutions

10:20: 10:40 **Ronen Zangi**
The Induced Interactions of Water

10:40-11:20 ***COFFEE BREAK AND POSTER SESSION***

Session IV: Chair E. Guàrdia

11:20-11:40 **José M. Soler**
Efficient van der Waals density functional simulations

11:40-12:00 **Fabiano Corsetti**
The structure of water from first-principles simulations with van der Waals interactions

12:00-12:20 **Pepa Cabrera-Sanfelix**
Water on surfaces from first-principles: binding and reactivity

12:20-12:40 **Paolo Nicolini**
Force matching algorithm: towards classical force fields for water with ab initio accuracy

12:40:13:00 **Rossend Rey**
Energy pathways for rotational relaxation in liquid water

13:00-13:30 ***DISCUSSION***