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 Cerdeiríña
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