

Poster presentations by participants

Tuesday, 6 October 2015 18:30 (1:30)

Content

Arevik Asatryan: Water induced helix-coil transition in biopolymers
Joel Baffour Awuah: First-principles Density Functional Theory study of Arsenic Immobilization by Al(III)-modified zeolite Clinoptilolite
José Rafael Bordin: Self-assembly and Waterlike Anomalies in Janus Nanoparticles
Ana Cunha: Structure and Dynamics and Water-Protein Interfaces
Hadeer A.K. El Habashy: On the Development of A Novel Bio-Molecular NanoSwitch; A Computational Approach
Konica Jannat Fatema: Determination of inorganic anions and cations in drinking water of Dhaka city by ion Chromatography and findout its health risk assessment
Piero Gasparotto: Probing defects and correlations in the hydrogen-bond network of water
Piero Gasparotto: Recognizing molecular patterns by machine learning: an agnostic structural definition of hydrogen bond
Chalernpol Kanchanawarin: Topic Structure and Dynamics of Water Molecules around POPE lipid bilayer using Molecular Dynamics Simulations
Fanimeh Maghsoodi: PEG-PCL Diblock Copolymers Self-Assembly to Nano-Structures Studied by Coarse-Grained Simulations
Pankaj K. Mishra: Ultrafast Energy Transfer from Solvent to Solute Induced by Sub-ps Highly Intensed THz Pulse
Tobias Morawietz: Simulating Proton Transfer Reactions in Liquid Water by Artificial Neural Networks
Maria Ortega Cruz: Hydration properties of single-stranded DNA films
Nurapati Pantha: Hydrophobicity of methane in different solvent environment: An enhanced sampling approach
Sergiy Perepelytsya: Dynamics and ordering of counterions in hydration shell of DNA double helix
Sunil Pokharel: Diffusion Coefficients of Nitric Oxide in Water: A molecular Dynamics
Acep Purqon: Free-Energy Analysis of the Preferred Configuration of Transmembrane Protein in Model Membrane: Roles of Lipid and Water
Jamileh Seyed Yazdi: Water Behavior at the Confined Volumes and Interfaces
Mohammad I. Siddiqi: Water-mediated pharmacophore-based identification of human Chk1 inhibitors as anti-cancer agents
Marina van der Merwe: Molecular dynamics simulations of a supersaturated salt solution
Ana Vila Verde: Additive and supra-additive slowdown of water rotation in aqueous electrolyte solutions
Chunlei Wang: Unexpected Hydrophobicity at Polar Surfaces

Summary

Session Classification : POSTER SESSION