

## Session Index

### Session L3: Focus Session: Solvation, Dynamics, and Reactivity in Complex Environments I

Sponsoring Units: DCP

Chair: Valeria Molinero, University of Utah

Room: 107

Wednesday, March 5, 2014 8:00AM - 8:12AM	<a href="#">L3.00001: Dynamic response in electric field-induced nanowetting in salt solution</a> Dusan Bratko , Davide Vanzo , Alenka Luzar
Wednesday, March 5, 2014 8:12AM - 8:24AM	<a href="#">L3.00002: First-principles investigation of boron incorporation into CRUD under Pressurized Water Reactor conditions</a> Zs. Rak , C.J. O'Brien , D.W. Brenner
Wednesday, March 5, 2014 8:24AM - 8:36AM	<a href="#">L3.00003: Atomistic Models for High-throughput Prediction of Hydration Free Energies</a> Jianzhong Wu
Wednesday, March 5, 2014 8:36AM - 9:12AM	<a href="#">L3.00004: Collisions of Sodium Atoms with Liquid Glycerol: Insights into Na Atom Solvation and Ionization and the Reactions of Near-Interfacial Electrons</a> Invited Speaker: Gilbert Nathanson
Wednesday, March 5, 2014 9:12AM - 9:24AM	<a href="#">L3.00005: Measurement of Ultraslow Rotational Dynamics of Probes in Imidazolium-Based Ionic Liquids Near and Below the Glass Transition Temperature: Studying the Role of Structural Heterogeneity on Dynamic Heterogeneity</a> Kayla Mendoza , Rakhitha Udugama-Arachchilage , Fehmi Bardak , George Tamas , Edward Quitevis
Wednesday, March 5, 2014 9:24AM - 9:36AM	<a href="#">L3.00006: CO2 capture in amine solutions from ab initio molecular dynamics</a> Changru Ma , Fabio Pietrucci , Wanda Andreoni
Wednesday, March 5, 2014 9:36AM - 9:48AM	<a href="#">L3.00007: \textit{Ab initio} Molecular Dynamics Study of Carbon Dioxide Adsorption on the Ni Catalyst Surface</a> Ji Il Choi , Yong-Hoon Kim
Wednesday, March 5, 2014 9:48AM - 10:24AM	<a href="#">L3.00008: Probing Intermolecular Interactions in Polycyclic Aromatic Hydrocarbons with 2D IR Spectroscopy</a> Invited Speaker: Amber Krummel
Wednesday, March 5, 2014 10:24AM - 10:36AM	<a href="#">L3.00009: Freezing and Melting of Salt Hydrates Next to Solid Surfaces Probed by Infrared-Visible Sum Frequency Generation Spectroscopy</a> Emmanuel Anim-Danso , Yu Zhang , Ali Dhinojwala
Wednesday, March 5, 2014 10:36AM - 10:48AM	<a href="#">L3.00010: Effects of Aqueous Solvation on the Photochemistry of Pyruvic Acid</a> Allison Reed-Harris , Barbara Ervens , Richard Shoemaker , Rebecca Rapf , Jay Kroll , Elizabeth Griffith , Anne Monod , Veronica Vaida
Wednesday, March 5, 2014 10:48AM - 11:00AM	<a href="#">L3.00011: Collisions and Reactions of HNO<sub>3</sub> and N<sub>2</sub>O<sub>5</sub> with Sea Spray Mimics</a> Michael Shaloski , Timothy Bertram , Gilbert Nathanson

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### Session Q3: Focus Session: Solvation, Dynamics, and Reactivity in Complex Environments II

Sponsoring Units: DCP

Chair: Francesco Paesani, University of California, San Diego

Room: 107

Wednesday, March 5, 2014 2:30PM - 3:06PM	<a href="#">Q3.00001: Water in Room Temperature Ionic Liquids</a> Invited Speaker: Michael Fayer
Wednesday, March 5, 2014 3:06PM - 3:18PM	<a href="#">Q3.00002: Comparative Study of the Intermolecular Dynamics of Benzene/Ionic Liquid Mixtures and Benzyl Functionalized Ionic Liquids: Femtosecond OKE Spectroscopic Measurements</a> Edward Quitevis , Lianjie Xue , George Tamas
Wednesday, March 5, 2014 3:18PM - 3:30PM	<a href="#">Q3.00003: Solvation dynamics in room temperature ionic liquids studied by ultrafast vibrational spectroscopy</a> Sean Garrett-Roe , Zhe Ren , Duane Couchot-Vore , Thomas Brinzer
Wednesday, March 5, 2014 3:30PM - 3:42PM	<a href="#">Q3.00004: Comparative Study of the Intermolecular Dynamics and Physical Properties of Branched and Linear Alkyl Chain Imidazolium Ionic Liquids</a> Lianjie Xue , Fehmi Bardak , George Tamas , Eshan Gurung , Edward Quitevis , Yung Koh , Sindee Simon
Wednesday, March 5, 2014 3:42PM - 4:18PM	<a href="#">Q3.00005: Structure and Dynamics of Nanoconfined Liquids</a> Invited Speaker: Ward Thompson
Wednesday, March 5, 2014 4:18PM - 4:30PM	<a href="#">Q3.00006: Confinement effects on collective water dynamics: Molecular dynamics study of optical Kerr response in silica nanopores</a> Anatoli Milischuk , Branka Ladanyi
Wednesday, March 5, 2014 4:30PM - 4:42PM	<a href="#">Q3.00007: A Molecularly-Based Theory for Electron Transfer in Polar Solvents</a> Bilin Zhuang , Zhen-Gang Wang
Wednesday, March 5, 2014 4:42PM - 4:54PM	<a href="#">Q3.00008: Polar nanoregions in water - a study of the dielectric properties of TIP4P/2005, TIP4P2005f and TTM3F</a> Daniel Elton , Marivi Fernandez-Serra
Wednesday, March 5, 2014 4:54PM - 5:06PM	<a href="#">Q3.00009: Systematic investigation of the electronic and structural properties of chloride ion in aqueous solution by advanced density functional</a> Arindam Bankura , Charles Swartz , Michael L. Klein , Xifan Wu
Wednesday, March 5, 2014 5:06PM - 5:18PM	<a href="#">Q3.00010: Relaxation Dynamics of the Solvated Electron in Water, Methanol and Ethanol</a> Madeline H. Elkins , Holly L. Williams , Daniel M. Neumark
Wednesday, March 5, 2014 5:18PM - 5:30PM	<a href="#">Q3.00011: Quantum diffusion of atomic hydrogen isotopes in water</a> David Bartels , Jonathan Walker

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### Session S2: Focus Session: Solvation, Dynamics, and Reactivity in Complex Environments III

Sponsoring Units: DCP

Chair: Christine Payne, Georgia Institute of Technology

Room: 102

Thursday, March 6, 2014 8:00AM - 8:12AM	<a href="#">S2.00001: Time-dependent density-functional theory for real-time electronic dynamics on material surfaces</a> Rulin Wang , Dong Hou , Xiao Zheng
Thursday, March 6, 2014 8:12AM - 8:24AM	<a href="#">S2.00002: The electrostatic double layer of Pt/water interfaces from first principles molecular dynamics</a> Clotilde Cucinotta , Pietro Ballone , Stefano Sanvito
Thursday, March 6, 2014 8:24AM - 8:36AM	<a href="#">S2.00003: Venturing into the kinetics and mechanism of nanoconfined solid-state reactions: Trimerization of sodium dicyanamide in nanopores</a> Benjamin Yancey , Sergey Vyazovkin
Thursday, March 6, 2014 8:36AM - 9:12AM	<a href="#">S2.00004: Water adsorption and proton conduction in metal-organic frameworks: Insights from molecular simulations</a> Invited Speaker: Francesco Paesani
Thursday, March 6, 2014 9:12AM - 9:24AM	<a href="#">S2.00005: Simulating and Modeling Transport Through Atomically Thin Membranes</a> Joseph Ostrowski , Joel Eaves
Thursday, March 6, 2014 9:24AM - 9:36AM	<a href="#">S2.00006: Theoretical analysis on ion transport through polymer networks in electrochemical capacitors</a> Jos W. Zwanikken , Yufei Jing , Vikram Jadhao , Charles E. Sing , Niels Boon , Monica Olvera de la Cruz
Thursday, March 6, 2014 9:36AM - 9:48AM	<a href="#">S2.00007: Direct simulation of proton-coupled electron transfer reaction dynamics and mechanisms</a> Joshua S. Kretchmer , Thomas F. Miller III
Thursday, March 6, 2014 9:48AM - 10:24AM	<a href="#">S2.00008: Wetting of hydrophobic and nanostructured surfaces</a> Invited Speaker: Alenka Luzar
Thursday, March 6, 2014 10:24AM - 10:36AM	<a href="#">S2.00009: Memory in 2D FT Spectra of Quantum Dots</a> Samuel Park , Dmitry Baranov , Byungmoon Cho , Trevor Courtney , David Jonas
Thursday, March 6, 2014 10:36AM - 10:48AM	<a href="#">S2.00010: First-principles study of single water interactions with the LaMnO<sub>3</sub> surface in the presence of defects, Sr substitution and varied surface morphologies</a> Chris Billman , Hai-ping Cheng
Thursday, March 6, 2014 10:48AM - 11:00AM	<a href="#">S2.00011: Nucleus-Coupled Electron Transfer Mechanism for TiO<sub>2</sub>-Catalyzed Water Splitting</a> Yiyang Sun , Michael Lucking , Damien West , Shengbai Zhang

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### Session W2: Focus Session: Solvation, Dynamics, and Reactivity in Complex Environments IV

Sponsoring Units: DCP

Chair: Ward Thompson, University of Kansas

Room: 102

Thursday, March 6, 2014 2:30PM - 3:06PM	<a href="#">W2.00001: Imaging and controlling intracellular reactions: Lysosome transport as a function of diameter and the intracellular synthesis of conducting polymers</a> Invited Speaker: Christine Payne
Thursday, March 6, 2014 3:06PM - 3:18PM	<a href="#">W2.00002: Myosin-II sets the optimal response time scale of chemotactic amoeba</a> Hsin-Fang Hsu , Christian Westendorf , Marco Tarantola , Eberhard Bodenschatz , Carsten Beta
Thursday, March 6, 2014 3:18PM - 3:30PM	<a href="#">W2.00003: Fluorescent Dendrimer Nanoconjugates as Advanced Probes for Biological Imaging</a> Daniel Reilly , Sung Hoon Kim , John A. Katzenellenbogen , Charles M. Schroeder
Thursday, March 6, 2014 3:30PM - 3:42PM	<a href="#">W2.00004: Preferential melting of secondary structures during protein unfolding in different solvents: Competition between hydrophobic solvation and hydrogen bonding</a> Biman Bagchi , Susmita Roy , Rikhia Ghosh
Thursday, March 6, 2014 3:42PM - 3:54PM	<a href="#">W2.00005: The \$gp41_{659-671}\$ HIV-1 antibody epitope: a structurally challenging small peptide</a> Yuan Zhang , Celeste Sagui
Thursday, March 6, 2014 3:54PM - 4:06PM	<a href="#">W2.00006: Solvation dynamics and enzyme catalysis in a designed enzyme undergoing directed evolution</a> Carl Schreck , Teresa Head-Gordon
Thursday, March 6, 2014 4:06PM - 4:18PM	<a href="#">W2.00007: Environmental Affects on Surfactin Studied Using Multidimensional Infrared Spectroscopy</a> Jacob Nite , Amber Krummel
Thursday, March 6, 2014 4:18PM - 4:54PM	<a href="#">W2.00008: Effect of surfaces in modulating protein folding mechanisms</a> Invited Speaker: Joan Shea
Thursday, March 6, 2014 4:54PM - 5:06PM	<a href="#">W2.00009: Solvation in Surfactant Films at the Water-Air Interface</a> Russell Perkins , Rebecca Rapf , Elizabeth Griffith , Veronica Vaida
Thursday, March 6, 2014 5:06PM - 5:18PM	<a href="#">W2.00010: Temperature Dependent Solvation Dynamics of the Chromophore Environment in the Far-Red Fluorescent Protein mPlum</a> Chola Regmi , Prem Chapagain , Bernard Gerstman
Thursday, March 6, 2014 5:18PM - 5:30PM	<a href="#">W2.00011: QTES-DFTB dynamics study on the effect of substrate motion on quantum proton transfer in soybean lipoxxygenase-1</a> James Mazzuca , Sophya Garashchuk , Jacek Jakowski

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### Session Y1: Focus Session: Solvation, Dynamics, and Reactivity in Complex Environments V

Sponsoring Units: DCP

Chair: Amber Krummel, Colorado State University

Room: 103/105

Friday, March 7, 2014 8:00AM - 8:36AM	<a href="#">Y1.00001: Weighted Random Mixing and Exact Finite Lattice Descriptions of Molecular Aggregation Equilibria</a> Invited Speaker: Dor Ben-Amotz
Friday, March 7, 2014 8:36AM - 8:48AM	<a href="#">Y1.00002: Rotational-Rate Heterogeneity in Polymers on the Picosecond and Second Timescales through 2D Kinetics</a> Mark Berg , Sachin Dev Verma , David Vanden Bout
Friday, March 7, 2014 8:48AM - 9:00AM	<a href="#">Y1.00003: Computer simulation study of structure and dynamics of supercooled water in silica nanopores</a> Nicholas Kuon , Branka Ladanyi
Friday, March 7, 2014 9:00AM - 9:12AM	<a href="#">Y1.00004: Electrolyte Structure near Electrode Interfaces in Lithium-Ion Batteries</a> Vincenzo Lordi , Mitchell Ong , Osvalds Verners , Adri van Duin , Erik Draeger , John Pask
Friday, March 7, 2014 9:12AM - 9:48AM	<a href="#">Y1.00005: Femtosecond optical force microscopy</a> Invited Speaker: Eric Potma
Friday, March 7, 2014 9:48AM - 10:00AM	<a href="#">Y1.00006: Spatio-spectral infrared vibrational nano-imaging of intermolecular coupling</a> Benjamin Pollard , Eric Muller , Markus Raschke
Friday, March 7, 2014 10:00AM - 10:12AM	<a href="#">Y1.00007: Synchrotron Infrared Nano-Spectroscopy</a> Eric Muller , Benjamin Pollard , Hans Bechtel , Michael Martin , Markus Raschke
Friday, March 7, 2014 10:12AM - 10:24AM	<a href="#">Y1.00008: Crystallization of supercooled liquids</a> Takashi Odagaki , Yuuna Shikuya
Friday, March 7, 2014 10:24AM - 11:00AM	<a href="#">Y1.00009: Single Molecule Approaches to Studying Heterogeneity in Molecular Supercooled Liquids</a> Invited Speaker: Laura Kaufman