

Agenda Friday, January 27th

8:30 am — Morning session begins in the Pelican Room

Session Chair: *Douglas Tobias Presiding*

8:30 to 9:10 — Beatriz Roldán Cuenya; “Structure, Chemical State, and Reactivity Investigations of Size- and Shape-Selected Nanocatalysts Under Operando Conditions”

9:10 to 9:30 — Amanda MacMillan, Theresa McIntire, J. Morrison, D. Tobias, S. Nizkorodov; “Interaction of Water Vapor with the Surfaces of Imidazolium Based Ionic Liquid Nanoparticles and Thin Films”

9:30 to 9:50 — Leon Phillips and D. Nesbitt; “The Solid Surface of Liquid Metals”

9:50 to 10:10 — Paul Nissenon, Lisa Wingen, D. Dabdub, B. Finlayson-Pitts; “Understanding the Formation of Bromine from Deliquesced Sodium Bromide Aerosol in the Presence of Ozone and UV Light”

10:10 to 10:40 — Break

Session Chair: *Sergey Nizkorodov Presiding*

10:40 to 11:00 — Christopher Mundy; “Ions at Interfaces: Molecular Simulation vs. Continuum Models”

11:00 to 11:20 — Crisand Anderson, Douglas Tobias, K. Callahan, N. Richards, B. Finlayson-Pitts; “The Effect of Cations on Nitrate Ion Photochemistry”

11:20 to 11:35 — Marcel Baer; “Theoretical Studies of HX (X = Cl, Br) at Interfaces”

11:35 to 11:55 — Alexander Laskin, R. Moffet, M. Gilles; “Tropospheric Chemistry of Internally Mixed Sea Salt and Organic Particles: Surprising Reactivity of NaCl with Weak Organic Acids”

11:55 to 1:15 — Catered lunch on the 15FiftyFive Terrace

Session Chair: *Filipp Furche Presiding*

1:15 to 1:55 — Heather Allen; “Ion and Lipid Organization at Air-Aqueous Interfaces”

1:55 to 2:15 — Martina Roeselová; “Molecular Dynamics Simulations of Lipid Films at the Air-Water Interface”

2:15 to 2:35 — Alla Zelenyuk, D. Imre, J. Beranek, M. Shrivastava; “On the Symbiotic Relation Between SOA and Hydrophobic Organics: SOA Evaporation, Kinetics, Phase, Morphology, Diffusivity, Viscosity, and Formation Yields”

2:35 to 2:50 — Break

Session Chair: *Leon Phillips Presiding*

2:50 to 3:10 — Matthew Dawson, Mychel Varner, V. Perraud, M. Ezell, A. Zelenyuk, B. Finlayson-Pitts, R. Gerber; “Formation and Properties of Particles from Methanesulfonic Acid and Amines”

3:10 to 3:25 — Barbara Cottrell, A. Tong, H. Santoke, B. Peake, W. van der Veer, A. Simpson, W. Cooper; “Time-Resolved Laser Flash Photolysis: Understanding the Photochemistry of Triplet State Dissolved Organic Matter (³CDOM*)”

3:25 to 3:40 — Enrico Tapavicza and F. Furche; “Non-Adiabatic Molecular Dynamics Simulations for Atmospheric Photochemistry”

3:40 to 3:50 — Concluding remarks; Matthew Platz and Zeev Rosenzweig

3:50 — Close of workshop; Barbara Finlayson-Pitts



Collaborative Workshop in Chemistry at Interfaces

*Eighth Annual Workshop
Surf and Sand Hotel
Laguna Beach, California
January 26-27, 2012*

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Agenda

Thursday, January 26th

8:30 am — Opening session begins in the Pelican Room

Barbara Finlayson-Pitts
Welcome and Introduction

Session Chair: *John Hemminger Presiding*

8:40 to 9:25 — Lara Gundel; “How Adapting to Global Warming May Influence Physical Chemistry at Indoor Surfaces”

9:25 to 9:45 — Abraham Stern, Barbara Finlayson-Pitts, S. Moussa, J. Raff, C. Dilbeck, D. Tobias; “Nitric Acid and Water on Organic Surfaces as a Proxy for Heterogeneous Chemistry in the Boundary Layer”

9:45 to 10:00 — Mychel Varner, B. Finlayson-Pitts, R. Gerber; “Reactions of N₂O₄ with Water”

10:00 to 10:15 — Henk Eshuis, R. Tran, F. Furche; “Formation of HONO from Excited NO₂ and Water in Ambient Air: A Density Functional and Multi-reference Theory Study”

10:15 to 10:30 — Poster summaries

10:30 to 11:30 — Break and poster session

Session Chair: *Donald Dabdub Presiding*

11:30 to 12:10 — Marsha Lester; “A New Spectroscopic Window on Hydroxyl Radicals and Their Association Reactions of Significance in the Atmosphere”

12:10 to 12:25 — Scott Epstein, D. Shemesh, V. Tran, S. Nizkorodov, R. Gerber; “Absorption Spectra and Photolysis of Methyl Peroxide in Liquid and Frozen Water”

12:25 to 1:45 — Catered lunch on the 15FiftyFive Terrace

Session Chair: *Benny Gerber Presiding*

1:45 to 2:25 — Branka Ladanyi; “Structure and Dynamics of Nanoconfined Water”

2:25 to 2:45 — Sotiris Xantheas, K. Kowalski, X.-B. Wang; “Joint First Principles Theoretical and Photoelectron Experimental Studies of Molecular and Aqueous Cluster Ions”

2:45 to 3:00 — Alexandria Margarella, K. Perrine, M. Faubel, B. Winter, J. Hemminger; “Investigation of the Dissociation of Sulfuric Acid Aqueous Solutions Using Photoelectron Spectroscopy”

3:00 to 3:15 — John Hemminger, T. Lewis, A. Margarella, M. Faubel, B. Winter; “Temperature Dependence of Nitric Acid Dissociation at the Interface and in the Bulk”

3:15 to 4:15 — Break and poster session

Session Chair: *Martina Roeselová Presiding*

4:15 to 4:55 — Valeria Molinero; “Crystallization of Water from the Bulk to the Nanoscale”

4:55 to 5:15 — Bernd Winter; “Charge and Energy Transfer in Aqueous Solution by Ionizing Radiation”

5:15 to 5:30 — Kathryn Perrine, A. Margarella, M. Faubel, B. Winter, J. Hemminger; “Photoelectron Spectroscopy Studies of Inhomogeneous Acetonitrile Solutions”

6:00 pm — Reception and dinner for invited speakers, faculty, international and DOE lab collaborators, and invited guests in the Top of the Surf Room

AFFILIATIONS OF COLLABORATORS, GUESTS, AND INVITED SPEAKERS

- Heather Allen: Ohio State University
- Marcel Baer: Pacific Northwest National Laboratory
- Barbara Cottrell: University of Toronto
- Beatriz Roldán Cuenya: University of Central Florida
- Lambert Doezema: Loyola Marymount University
- Jean Futrell: Pacific Northwest National Laboratory
- Bruce Garrett: Pacific Northwest National Laboratory
- Lara Gundel: Lawrence Berkeley National Laboratory
- Timothy Killeen: National Science Foundation
- Branka Ladanyi: Colorado State University
- Alexander Laskin: Pacific Northwest National Laboratory
- Marsha Lester: University of Pennsylvania
- Valeria Molinero: University of Utah
- Christopher Mundy: Pacific Northwest National Laboratory
- Paul Nissenon: California State Polytechnic University, Pomona
- Leon Phillips: University of Canterbury, New Zealand
- Matthew Platz: National Science Foundation
- Martina Roeselová: Academy of Sciences, Czech Republic
- Zeev Rosenzweig: National Science Foundation
- Bernd Winter: BESSY Institute, Germany
- Sotiris Xantheas: Pacific Northwest National Laboratory
- Alla Zelenyuk: Pacific Northwest National Laboratory