

8:30 am — Morning session begins in the Sand Dollar Room

Barbara Finlayson-Pitts: Announcements

Session Chair: *Doug Tobias Presiding*

8:35 to 9:15 — Anne McCoy; “How Large Amplitude Motions in Atmospheric and Astrochemical Molecules are Reflected in Their Spectra”

9:15 to 9:35 — Jaroslav Kalinowski, M. Rasanen, R.B. Gerber; “Decomposition and Reaction Dynamics of Criegee Intermediates”

9:35 to 9:55 — Evangelos Miliordos and Sotiris Xantheas; “Biradical Species: Their Characterization and Importance in Atmospheric Particle Formation”

9:55 to 10:45 — Break and poster session in the Sand Castle Room

Session Chair: *Benny Gerber Presiding*

10:45 to 11:05 — Jordan Vincent, Ben Toulson, C. Murray, F. Furche; “Probing Methylamine Photochemistry by Velocity-Map Ion Imaging and Non-Adiabatic Molecular Dynamics Simulations”

11:05 to 11:45 — Scot Martin; “Heterogeneous Chemistry Leading to SOA Production During Isoprene Oxidation”

11:45 to 12:00 — Hyun Ji (Julie) Lee, P. Aiona, D. Romonosky, R. Leslie, A. Laskin, J. Laskin, S. Nizkorodov; “Photochemical Cloud Processing of Light-Absorbing Organic Aerosols”

12:00 to 12:15 — Scott Epstein and Sergey Nizkorodov; “Photochemistry in Atmospheric Condensed Phases: Effect on Aerosol Concentration and Chemical Composition”

12:15 to 2:00 — Catered lunch on the 15FiftyFive Terrace

Session Chair: *Donald Dabdub Presiding*

2:00 to 2:20 — Alex Laskin, J. Laskin, S. Nizkorodov, et al.; “Molecular Characterization of Brown Carbon—What Can be Learned and How?”

2:20 to 2:40 — Alla Zelenyuk, D. Imre, M. Shrivatsa, E. Abramson, L. Kleinman, J. Fast, S.S. Springston; “New, Experimentally Based Secondary Organic Aerosol Paradigm Removes Discrepancies Between Models and Data: Revisiting Mexico City SOA Data”

2:40 to 2:55 — Carla Kidd, V. Perraud, L. Wingen, B.J. Finlayson-Pitts; “Integrating Phase and Composition of Secondary Organic Aerosol from the Ozonolysis of α -Pinene”

2:55 to 3:35 — Murray Johnston; “Chemical Composition of Ambient Nanoparticles”

3:35 to 4:05 — Haihan Chen, Mychel Varner, Matthew Dawson, Andrew Martinez, V. Perraud, K. Arquero, A. Gomez, R.B. Gerber, D. Dabdub, B. J. Finlayson-Pitts; “Particles and Their Precursors: From Angstrom to Regional Scales”

4:05 to 4:20 — Zeev Rosenzweig; “Some Comments from a Long-Time Observer”

4:20 — Close of workshop; Barbara Finlayson-Pitts

5:30-6:00 pm — Dinner for invited speakers, faculty, international and DOE lab collaborators, and invited guests at Las Brisas Restaurant, located at 361 Cliff Drive (at the corner of Pacific Coast Highway)



Collaborative Workshop in Chemistry at Interfaces

*Tenth Annual Workshop
Surf and Sand Hotel
Laguna Beach, California
January 22 – 23, 2014*

*Funded by NSF
University of California, Irvine
www.airuci.uci.edu*

8:30 am — *Opening session begins in the Sand Dollar Room*
Barbara Finlayson-Pitts: Welcome and Introduction

Session Chair: John Hemminger Presiding

8:40 to 9:20 — David Nesbitt; “Fishing for Excess Ions at the Gas-Liquid Interface: A Quantum State-Resolved Approach”

9:20 to 9:40 — Sampsa Riikonen, L. Halonen, R.B. Gerber; “Ionization of Acids at the Liquid-Like Layer on Ice”

9:40 to 10:00 — Chris Mundy, M. Baer, A. Stern, D.J. Tobias; “Ten Years of Simulating the Air-Water Interface: Past, Present, and Future”

10:00 to 10:15 — Poster summaries

10:15 to 11:00 — *Break and poster session in the Sand Castle Room*

Session Chair: Craig Murray Presiding

11:00 to 11:20 — Evangelos Miliordos and Sotiris Xantheas; “The Mechanism Behind the Stabilization of Multi-Charged Cations in an Aqueous Environment: Relative Shifts of the Various Electronic States During Microhydration of Mg²⁺, Ca²⁺, Fe²⁺, Al³⁺ and Fe³⁺”

11:20 to 11:40 — Abe Stern, Kathryn Perrine, M. Van Spyk, J.C. Hemminger, D.J. Tobias; “Specific Cation Effects on Halide Ion Adsorption to the Air-Water Interface: XPS and MD Simulation Studies”

11:40 to 11:55 — Krista Parry, A. Stern, J.C. Hemminger, D.J. Tobias; “Toward Direct Comparison of Ion Distributions at the Air-Water Interface from XPS Data and MD Simulations”

11:55 to 1:30 — *Group photo, catered lunch on the 15FiftyFive Terrace*

Session Chair: Sergey Nizkorodov Presiding

1:30 to 2:10 — Vicki Grassian; “Toward a Greater Understanding of the Atmospheric Chemistry and Impacts of Mineral Dust and Sea Spray Aerosols Through Laboratory Studies”

2:10 to 2:30 — Garold Murdachaew, M.P. Gaigeot, L. Halonen, R.B. Gerber; “Acid Ionization on Wet Silica”

2:30 to 3:10 — Martina Havenith; “Solvation—New Insights by THz Spectroscopy”

3:10 to 3:30 — Bernd Winter, T. Lewis, S. Thürmer, R. Seidel, D.J. Tobias, J.C. Hemminger; “Organosulfur Aqueous Solutions: How Photoelectron Angular Distributions Connect to Molecular Surface Adsorption”

3:30 to 4:15 — *Break and poster session in the Sand Castle Room*

Session Chair: Filipp Furche Presiding

4:15 to 4:35 — Scott Hollingsworth, Theresa McIntire, A. Stern, J.C. Hemminger, D.J. Tobias; “Vibrational Spectroscopy of Water in Defects of SAMs”

4:35 to 4:55 — Michael Makowski, A. Stern, Kathryn Perrine, M. Van Spyk, B. Winter, J.C. Hemminger, D.J. Tobias; “Concentration-Dependent Distribution and Orientation of Acetonitrile at the Air-Water Interface”

4:55 to 5:15 — Martina Roeselová; “Mixed Aromatic-Aliphatic Films at the Air-Water Interface”

6:00 pm — *Dinner for all workshop attendees in the Pelican Room*

AFFILIATIONS OF COLLABORATORS, GUESTS, AND INVITED SPEAKERS

- Donald Baer: Pacific Northwest National Laboratory
- Marcel Baer: Pacific Northwest National Laboratory
- Allison Campbell: Pacific Northwest National Laboratory
- Lambert Doezema: Loyola Marymount University
- Jean Futrell: Pacific Northwest National Laboratory
- Vicki Grassian: University of Iowa
- Audrey Hammerich: University of Illinois, Chicago
- Martina Havenith: Ruhr-University Bochum; Germany
- Murray Johnston: University of Delaware
- Jaroslaw Kalinowski: University of Helsinki, Finland
- Alexander Laskin: Pacific Northwest National Laboratory
- Theresa Longin: University of Redlands
- Scot Martin: Harvard University
- Anne McCoy: The Ohio State University
- Evangelos Miliordos: Pacific Northwest National Laboratory
- Christopher Mundy: Pacific Northwest National Laboratory
- Garold Murdachaew: University of Helsinki, Finland
- David Nesbitt: University of Colorado, Boulder
- Paul Nissenon: California State Polytechnic University, Pomona
- Leon Phillips: University of Canterbury, New Zealand
- Sampsa Riikonen: University of Helsinki, Finland
- Martina Roeselová: Academy of Sciences, Czech Republic
- Zeev Rosenzweig: University of Maryland
- Bernd Winter: Helmholtz Zentrum Berlin, Germany
- Sotiris Xantheas: Pacific Northwest National Laboratory
- Alla Zelenyuk: Pacific Northwest National Laboratory



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