

AGENDA Thursday, January 20th

9:00 am — Morning session begins

Session Chair: *John Hemminger Presiding*

9:00 to 9:40 — Joe Francisco; “Catalytic Effect of Water Molecules on Atmospheric Reactions”

9:40 to 10:00 — Sotiris Xantheas; “Water Mediated Peptide-Peptide Interaction and the Role of Hydrophobicity”

10:00 to 10:20 — Matt Dawson, Mychel Varner, V. Perraud, M. Ezell, R. Gerber, M. Kleinman, B. Finlayson-Pitts; “Effects of Water on Nanoparticle Formation from Methanesulfonic Acid: Approaching the Limit of Interfaces in Complex Systems”

10:20 to 10:35 — Zenghui Yang, Henk Eshuis, F. Furche; “Atmospheric HONO Generation from Excited NO₂ and Water: A Computational Study”

10:35 to 11:00 — Break

Session Chair: *Filipp Furche Presiding*

11:00 to 11:15 — Hanna Lignell, A. Hammerich, B. Finlayson-Pitts, R. Gerber; “Isomerization and Ionization of N₂O₄ on Ice and Silica Surfaces”

11:15 to 11:30 — Noriko Nishino, M. Ezell, S. Johnson, V. Perraud, B. Finlayson-Pitts; “Thermal and Photochemical Reactions of Oxides of Nitrogen on Cr₂O₃”

11:30 to 11:50 — John Hemminger, Abe Stern, T. Lewis, B. Winter, M. Faubel, C. Mundy, M. Baer, D. Tobias; “Bulk vs Interfacial HNO₃(aq): XPS Experiments and First-Principles Molecular Dynamics Simulations”

11:50 to 12:05 — Tanza Lewis, T. Kahan, D. Tobias, M. Faubel, B. Winter, J. Hemminger; “In-Situ XPS Studies of the Liquid/Vapor Interface of Aqueous Solution: CO₂ Capture in Aqueous Monoethanolamine (MEA) Solutions and Surface Propensity of Aqueous Organosulfur Compounds”

12:05 to 1:30 — Catered lunch

Session Chair: *Sergey Nizkorodov Presiding*

1:30 to 1:45 — Tara Kahan, J. Vincent, D. Donaldson, J. Hemminger, D. Tobias; “Interactions of Hydroxyl Radicals with Liquid and Frozen Water”

1:45 to 2:05 — W. Pfalzgraff, S. Neshyba, Martina Roeselová; “Structure and Dynamics of the Quasi-Liquid Layer at Basal, Prismatic, and Pyramidal Surfaces of Ice”

2:05 to 2:25 — Christopher Mundy; “Re-Examining the Specific Ion Effect with Density Functional Theory”

2:25 to 2:45 — Will Kuo; “Interfacial Effect on Molecular Decomposition via SN₂ Reaction”

2:45 to 3:05 — Nicole Richards, Carol Tsai, K. Callahan, L. Wingen, N. Nishino, M. Kleinman, D. Tobias, B. Finlayson-Pitts; “Effects of Mixed Chloride/Bromide Ions on Nitrate Ion Photochemistry”

3:05 to 3:25 — Paul Nissenon, Lisa Wingen, S. Hunt, B. Finlayson-Pitts, D. Dabdub; “The Dynamics of Molecular Bromine Formation from NaBr Aerosols”

3:25 to 3:35 — Concluding remarks and impressions: Zeev Rosenzweig; National Science Foundation

3:35 to 3:40 — Close of workshop: Barbara Finlayson-Pitts



*Collaborative Workshop in
Chemistry at the Interfaces*

Seventh Annual Workshop

Surf and Sand Hotel

Laguna Beach, California

January 19-20, 2011

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AGENDA Wednesday, January 19th

8:30 am — *Opening session begins*

Barbara Finlayson-Pitts, AirUCI Director

Welcome and Introduction

Session Chair: Doug Tobias Presiding

8:45 to 9:25 — Günter Oberdörster; “Airborne Nano-Sized Particles and the Central Nervous System”

9:25 to 9:45 — Michael Dennin and T. Boatwright; “Using Langmuir Monolayers to Study Particle-Membrane Interactions”

9:45 to 10:00 — Jordan Vincent and D. Tobias; “Coarse-grained Molecular Dynamics Simulations of Nanoparticle Interactions with Lipid Bilayers and Monolayers”

10:00 to 10:20 — Michael Kleinman, G. Gookin, A. Keebaugh, L. Mendez, B. Finlayson-Pitts, Lisa Wingen; “Compositions and Size Distributions of Fine and Ultrafine Particles and their Effects on Health”

10:20 to 10:50 — *Break and group photo*

Session Chair: Donald Dabdub Presiding

10:50 to 11:30 — Laurie Butler; “OH-Initiated Oxidation of Volatile Organic Compounds: Dynamics of the OH + Ethene Reaction”

11:30 to 11:45 — Adam Bateman, S. Nizkorodov, J. Laskin, A. Laskin; “Photochemical Cloud Processing of Biogenic Secondary Organic Aerosol”

11:45 to 12:05 — Alex Laskin, J. Laskin, P. Roach, S. Nizkorodov, D. Bones, T. Nguyen, A. Bateman; “Molecular Characterization of N-Containing Constituents in Laboratory and Ambient Samples of Organic Aerosol”

12:05 to 12:20 — Henk Eshuis, H. S. Kim, S. Nizkorodov, F. Furche; “Computational Clues on the Brown Color of Secondary Organic Aerosols”

12:20 to 1:30 — *Catered lunch*

Session Chair: Leon Phillips Presiding

1:30 to 2:10 — Allan Bertram; “The Physical State of Atmospheric Particles Can Be Predicted with Parameters that are Now Measured Worldwide”

2:10 to 2:30 — Alla Zelenyuk, T. Vaden, J. Beránek, M. Shrivastava, J. Fast, D. Imre; “On the Evaporation Kinetics and Phase of Laboratory and Ambient Secondary Organic Aerosol”

2:30 to 2:45 — Emily Bruns, J. Greaves, B. Finlayson-Pitts; “Measuring Vapor Pressures and Heats of Vaporization Using ASAP”

2:45 to 3:00 — Tran Nguyen, S. Nizkorodov, P. Roach, A. Laskin, J. Laskin; “Effects of NO_x and Relative Humidity on the Molecular Composition of Isoprene Aerosol”

3:00 to 3:15 — Barbara Cottrell, E. Bruns, J. Greaves, S. Nizkorodov, W. Cooper, B. Finlayson-Pitts, A. Simpson; “Characterizing Rainwater Dissolved Organic Matter: Is “Humic-Like” an Accurate Representation?”

3:15 to 3:30 — Wayne Chang, A. Miguel, L. Doezema, D. Dabdub; “Contribution of Polycyclic Aromatic Hydrocarbons to Aerosol Burdens in Southern California”

3:30 to 4:00 — *Break*

Session Chair: Martina Roeselová Presiding

4:00 to 4:40 — John Stanton; “Calculating Accurate Vibrational Energy Levels: Quantum Chemistry, the Nuclear Motion Hamiltonian, and Practical Considerations”

4:40 to 4:55 — Matthias Heyden, G. Niehues, S. Funkner, D. Schmidt, G. Schwaab, K. Callahan, M. Havenith, D. Tobias; “Ions in Motion: The Intermolecular Vibrations of Solvated Ions in the Far Infrared”

4:55 to 5:15 — D. Packwood and Leon Phillips; “Non-Equilibrium Thermodynamics of the Air-Sea Exchange of Carbon Dioxide”

6:30 pm — *Dinner for invited speakers, faculty, international and DOE lab collaborators, and invited guests at Las Brisas restaurant.*

❖ *Meet at valet parking stand at 5:45 for carpooling.*

AFFILIATIONS OF COLLABORATORS AND GUEST SPEAKERS

- Donald Baer: Pacific Northwest National Laboratory
- Allan Bertram: University of British Columbia
- Laurie Butler: University of Chicago
- Allison Campbell: Pacific Northwest National Laboratory
- Joseph Francisco: Purdue University
- I-Feng Kuo: Lawrence Berkeley National Laboratory
- Alexander Laskin: Pacific Northwest National Laboratory
- Christopher Mundy: Pacific Northwest National Laboratory
- Günter Oberdörster: University of Rochester
- Leon Phillips: University of Canterbury, New Zealand
- Martina Roeselová: Academy of Sciences, Czech Republic
- Zeev Rosenzweig: National Science Foundation
- John Stanton: University of Texas, Austin
- Sotiris Xantheas: Pacific Northwest National Laboratory
- Alla Zelenyuk: Pacific Northwest National Laboratory