

**“A little insight goes a long way: a transformative role of theory in spectroscopy and chemical dynamics.”**

## **A symposium in honor of Prof. Benny Gerber**

“The purpose of computing is insight, not numbers”

R.W. Hamming

The symposium will highlight a transformative role that theory plays in modern research by making bold predictions, guiding the design of new experiments, and enabling insightful interpretation of experimental observations. The focus of the symposium will be on the theories and computational approaches connecting experimental observations to the underlying interactions between atoms and molecules developed by Prof. Benny Gerber and his colleagues, collaborators, students, and post docs. The topics will cover a broad range of experimental and theoretical physical chemistry including atmospheric processes, novel rare gas containing compound, new spectroscopic approaches, and more.

### **Symposium sponsors:**

Fritz Haber Center (The Hebrew University of Jerusalem)  
University of California, Irvine  
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### **Preliminary program:**

The symposium is a part of ACS National Meeting in Dallas, March 16-20, 2014. We are scheduled for Sunday, Monday, and Wednesday (Tuesday is reserved for ACS award symposia).

On Monday evening, a hosted symposium reception and dinner is planned.

### **Session I: Biology and condensed phase (Sunday AM)**

Chair: Anna Krylov

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|----------------|---------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>810-815</b> | Welcome remarks                                                                                                                                   |
| <b>815-845</b> | <u>Doug Tobias</u> , “Making sense of transmembrane voltage sensing by voltage-gated ion channels: concerted simulation and experimental studies” |
| <b>845-915</b> | <u>Pavel Jungwirth</u> , “Photoionization in water: Electrons, cationic holes, and DNA damage”                                                    |
| <b>915-945</b> | <u>Ron Elber</u> , “Overcoming the time scale gap of molecular dynamics”                                                                          |

- 945-1000 break
- 1000-1030 Benny Gerber, "Structure and structural transitions of charged proteins in mass spectrometry"
- 1030-1100 Yifat Miller "Self-assembly of peptides: Design of novel peptides for biotechnology applications and insight into amyloidogenic diseases"
- 1100-1130 Max Berkowitz, "Interaction of antimicrobial peptides with lipid bilayers"
- 1130-1200 Adrian Roitberg, "How Benny got hooked into biomolecules and other adventures"

### Session II: Non-adiabatic dynamics (Sunday PM)

Chair: Pavel Jungwirth

- 1330-1400 Anna Krylov, "Fission of entangled spins: An electronic structure perspective"
- 1400-1430 Bob Cave, "Block diagonalization approach to diabatic EOM-CC states"
- 1430-1500 Ryan Steele, "Signatures of nuclear and electronic motion in oxidized water clusters"
- 1500-1530 Mitchio Okumura, "Dynamics at conical intersections: Threshold Photoelectron-Photoion Coincidence (T-PEPICO) spectroscopy of the nitrate cation  $\text{NO}_3^+$ "
- 1530-1545 break
- 1545-1615 Bill Miller, "Symmetrical windowing for quantum states in quasi-classical trajectory simulations; application to electronically non-adiabatic processes"
- 1615-1645 Ara Apkarian, "Reality check of insights: Imaging motion, from ensembles to single molecules"
- 1645-1715 Mark Ratner, "Some transport science for Benny"

### Session III: New frontiers in methodology (Monday AM)

Chair: Ryan Steele

- 815-845 Mark Gordon, "Water and stuff in it"
- 845-915 Roi Baer, "Self-averaging stochastic Kohn-Sham density functional theory and extensions"
- 915-945 Curt Wittig, "Darwin term"
- 945-1000 break
- 1000-1030 Rob Coalson, "Simulations and statistical mechanical models of selectivity in the nuclear pore complex"
- 1030-1100 Nancy Makri, "Quantum-classical path integral: Methodology and application to charge transfer in solution"
- 1100-1130 Joel Bowman, "A simple Gerberian theory of mode-specific tunneling with applications"
- 1130-1200 Abraham Nitzan "Spectroscopic manifestations of inelastic tunneling in molecular conduction junctions"

### Session IV: Spectroscopy (Monday PM)

Chair: Ara Apkarian

- 1330-1400** Anne McCoy, "Using diffusion Monte Carlo to investigate rotations and vibrations in molecules that exhibit large amplitude motions"
- 1400-1430** Jim Anderson, "Interplay of experiment and theory for the hydrogen/iodine reaction"
- 1430-1500** Ned Sibert, "Alkyl CH stretch vibrations as a probe of conformational preferences"
- 1500-1530** Marie-Pierre Gaigeot, "DFT-MD simulations for vibrational spectroscopy: a little insight into finite temperature spectroscopy and anharmonicities"
- 1530-1545** break
- 1545-1615** Zlatko Bacic, "Hydrogen molecules in nanoscale cavities: Quantum dynamics, inelastic neutron scattering spectroscopy, and a new selection rule for H<sub>2</sub> in C<sub>60</sub>"
- 1615-1645** Piotr Piecuch, "Understanding photochemistry and photo-ionization dynamics with highly correlated electronic structure methods: Two examples that highlight the transformative role of theory in the interpretation of experimental observations"
- 1645-1715** Dan Neumark, "Spectroscopy of cryogenically-cooled anions by slow electron velocity-map imaging"

### **Session V: Atmospheric Chemistry (Wednesday AM)**

Chair: Anne McCoy

- 815-845** Barbara Finlayson-Pitts, "The essential role of theory in understanding atmospheric reactions"
- 845-915** Jaroslav Kalinowski, "Nature, isomerization and decomposition of a Criegee Intermediate: Dynamics using a multireference potential"
- 915-945** Sergei Nizkorodov, "Combined experimental and theoretical studies of photolysis of atmospherically relevant organic compounds in various phases"
- 945-1015** Mychel Varner, "Intermediates in the photooxidation of ammonia"
- 1015-1030** break
- 1030-1100** Garold Murdachaew, "Dissociation of HCl into ions on wet hydroxylated (0001) alpha-quartz"
- 1100-1130** Martina Roeselova, "Haloalkanes at air-water and air-ice interfaces: A computational study with implications in atmospheric chemistry and water treatment"
- 1130-1200** Veronica Vaida, "Water in thermal and photochemical multiphase atmospheric chemistry"

### **Session VI: Novel Compounds and interesting chemistry (Wednesday PM)**

Chair: Sergei Nizkorodov

- 1330-1400** George Schatz, "Studies of gas-surface interactions and of ions at liquid surfaces"

- 1400-1430** Jan Lundell, "From computer experiments to noble chemistry: The noble gas hydrides"
- 1430-1500** Markku Räsänen, "Chemical bonding and interactions of noble-gas species"
- 1500-1530** Barak Hirshberg, "Theoretical prediction of crystalline N<sub>8</sub>"
- 1530-1545** break
- 1545-1615** Sotiris Xantheas, "Analysis of bonding patterns in molecular systems exhibiting partial biradical character"
- 1615-1645** Dorit Shemesh, "Dynamics of triplet state photochemistry of aldehydes"
- 1645-1715** Gil Nathanson, "Exploring collisions and reactions between gases and high vapor pressure liquids"