



Department of Chemistry, March 2011

**POSTDOCTORAL SCHOLAR POSITIONS  
THEORETICAL AND COMPUTATIONAL CHEMICAL PHYSICS**

RESEARCH TOPICS:

**(A) Computational Biophysics**

Simulation of amyloid fibril structures and aggregation kinetics, lipid-protein complexes and antibody interactions and how they can be probed by novel multidimensional spectroscopy ranging from the infrared to the ultraviolet.

**(B) Attosecond X-ray Spectroscopy of Molecules**

Developing time-dependent many-body approaches to nonlinear x-ray core-electron spectra and their description in terms of real-space and real-time wavepackets of electrons and nuclei. Computational tools will be implemented for the design and analysis of measurements involving multiple ultrafast optical and x-ray pulses.

**(C) Energy and charge separation in photosynthetic complexes studied by nonlinear spectroscopy**

Developing and applying time-dependent density functional, nonequilibrium Green's Function techniques and exciton models for computing electronic excitations of molecular assemblies, light harvesting complexes and current-carrying molecules. Connection is made to quantum information processing and manipulation.

**(D) Nonlinear Spectroscopy with Quantum Optical Fields**

New optical signals which use entangled photons, pulse shaping, and coherent control algorithms are designed and simulated for probing molecular relaxations and exciton transport.

Ph.D. is required. Salary will commensurate with experience. Send a curriculum vitae, publication list and arrange for three letters of recommendation to be sent to:

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1. "Coherent Multidimensional Optical Probes for Electron Correlations and Exciton Dynamics; from NMR to X-rays", S. Mukamel, D. Abramavicius, L. Yang, W. Zhuang, I.V. Schweigert and D. Voronine. *Acct.Chem.Res.* 42, 553-562 (2009).
2. "Coherent Multidimensional Optical Spectroscopy Excitons in Molecular Aggregates; Quasiparticle vs. Supermolecule Perspectives", D. Abramavicius, B. Palmieri, D. Voronine, F. Sanda and S. Mukamel, *Chem. Rev.* 109, 2350-2408 (2009).
3. "Coherent Multidimensional Vibrational Spectroscopy of Biomolecules; Concepts, Simulations and Challenges". W. Zhuang, T. Hayashi and S. Mukamel, *Agnew Chem. Int.Ed.* 48, 3750-3781 (2009).
4. "Coherent Ultrafast Core-hole Correlation Spectroscopy: X-ray Analogues of Multidimensional NMR" I. V.Schweigert and S. Mukamel, *Phys. Rev. Lett.* 99, 163001 (2007).
5. "Ultrafast Double-Quantum Coherence Spectroscopy of Exciton with Entangled Photons", M. Richter and S. Mukamel, *Phys. Rev. A.* 82, 013820 (2010).
6. "Signatures of Quasiparticles Entanglement in Multidimensional Nonlinear Optical Spectroscopy of Aggregates", S. Mukamel, *J. Chem.Phys.* 132, 241105 (2010).
7. "Multidimensional Attosecond Photoelectron Spectroscopy with Shaped Pulses and Quantum Optical Fields", S. Rahav and S. Mukamel, *Phys. Rev. A.* 81,063810 (2010).

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