



Department of Chemistry, November 2012

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

RESEARCH TOPICS:

(A) 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.

(B) 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 exciton dynamics in molecular aggregates and semiconductor nanostructures.

(C) Many Body Theory of Nonlinear Response in the Condensed Phase

Developing and applying time-dependent density functional, nonequilibrium Green's Function techniques and exciton models for computing electronic excitations of molecular assemblies, energy and charge separation in photosynthetic complexes and current-carrying molecules. Connection to quantum information processing and manipulation will be explored.

(D) 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.

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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Relevant Publications

1. "Entangled Valence Electron-hole Dynamics Revealed by Stimulated Attosecond X-ray Raman Scattering", D. Healion, Y. Zhang, J.D. Biggs, N. Govind, and S. Mukamel. *J. Phys. Chem. Lett.* 3, 2326-2331 (2012)
2. "Heat Fluctuations and Coherences in a Quantum Heat Engine", S. Rahav, U. Harbola and S. Mukamel. *Phys Rev. A.* 86, 043843(2012).
3. "Photon Coincidence Counting in Parametric Down Conversion; Interference of Field-Matter Quantum Pathways", K. Dorfman and S. Mukamel. *Phys. Rev. A*, 86, 023805 (2012).
4. "Quantum Field, Interference, and Entanglement Effects in Nonlinear Optical Spectroscopy", S. Mukamel and Y. Nagata, *Procedia. Chem.* 3, 132-151(2011).
5. "Ultrafast Nonlinear Optical Signals Viewed from the Molecules Perspective; Kramers-Heisenberg Transition Amplitudes vs. Susceptibilities", S. Rahav and S. Mukamel, *Advances in Atomic Molecular and Optical Physics*, Vol. 59, Pages 223-263, (2010).
6. "Multidimensional Attosecond Photoelectron Spectroscopy with Shaped Pulses and Quantum Optical Fields", S. Rahav and S. Mukamel, *Phys. Rev. A.* 81,063810 (2010).
7. "Two Dimensional Ultraviolet (2DUV) Spectroscopic Tools for Identifying Fibrillation Propensity of Protein Residue Sequences", J. Jiang and S. Mukamel, *Angewandte Chemie Int. Ed.* 49, 9666-9669 (2010).
8. "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).
9. "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).