August 2018

4 POSTDOCTORAL POSITIONS
THEORY AND SIMULATION OF ULTRAFAST NONLINEAR X-RAY SPECTROSCOPY OF MOLECULES

Emerging X-ray free electron laser (XFEL) beam sources offer new types of probes of matter with unprecedented spatial and temporal resolutions. This research program funded by the US Department of Energy (DOE) aims at developing cutting- edge theoretical and simulation tools for nonlinear multidimensional X-ray/optical spectroscopies. 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 will be developed. Computational tools will be implemented for the design and analysis of measurements involving multiple ultrafast optical and X-ray pulses. Predictive modeling of these novel measurements requires the combination of analytical theory for nonlinear interactions of light and matter, robust quantum-chemical methodologies for the accurate description of electronic structure of various materials, and multiscale *ab initio* electron and nuclear dynamics techniques operating beyond Born-Oppenheimer approximation.

This multi-disciplinary research program will be carried out by a four-institution research team (UC Irvine, University of Bologna, PNNL and LANL), which spans the broad and necessary expertise in theoretical spectroscopy, nonlinear optics, quantum chemistry. We intend to fill 4 postdoctoral positions, each position will be based in one of participating institutions. Postdocs will have the opportunity to closely interact with, visit the other labs, and work closely with ongoing experiments.

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Desired Skills:

- Experience with scientific programming (MPI, Fortran, Python, C++)
- Demonstrated ability to work independently and with minimum supervision.
- Ability to adapt to new requirements for projects and be flexible enough to learn new areas of research as needed.
- Ability to work effectively as a part of a team in a multi-disciplinary multi-institution environment and interact with people with a variety of expertise

To apply for all positions: please send your CV and cover letter to Professor Shaul Mukamel and arrange 3 letters of recommendation to be emailed.

Indicate your preferences among the four groups. Salary will be commensurate with experience.

Recent Publications

1. *"Monitoring Nonadiabatic Avoided Crossing Dynamics in Molecules by Ultrafast X-Ray Diffraction", Markus Kowalewski, Kochise Bennett, and Shaul Mukamel. Structural Dynamics, 4, 054101 (2017)*
2. *"A quantum chemical interpretation of two-dimensional electronic spectroscopy of Light-Harvesting complexes", Segatta, Francesco; Cupellini, Lorenzo; Jurinovich, Sandro; Mukamel, Shaul; Dapor, Maurizio; Taioli, Simone; Garavelli, Marco; Mennucci, Benedetta. J. Am. Chem. Soc., (2017), 139 (22), 7558-7567.*
3. *"Simulating Coherent Multidimensional Spectroscopy of Nonadiabatic Molecular Processes; from the Infrared to the X-ray Regime", ", Markus Kowalewski ,Benjamin Fingerhut, Konstantin Dorfman, Kochise Bennett and Shaul Mukamel. Chem. Rev., 2017, 117 (19), pp 12165–12226*
4. *"Multidimensional Resonant Nonlinear Spectroscopy with Coherent Broadband X-ray Pulses", Kochise Bennett, Yu Zhang, Markus Kowalewski, Weijie Hua, and Shaul Mukamel. 2016 Phys. Scr. T169, 014002*
5. *"Catching Conical Intersections in the Act; Monitoring Transient Electronic Coherences by Attosecond Stimulated X-ray Raman Signals", Markus Kowalewski, Kochise Bennett, Konstantin Dorfman, and Shaul Mukamel. Phys. Rev. Lett. 115, 193003 (2015)*
6. *"Light-Driven and Phonon-Assisted Dynamics in Organic and Semiconductor Nano-Structures" Svetlana Kilina, Dmitri Kilin, and Sergei Tretiak, Chem. Rev., 115, 5929 – 5978 (2015).*
7. *"Coherent Exciton-Vibrational Dynamics and Energy Transfer in Conjugated Organics", T. R. Nelson, D. Ondarse-Alvarez, N. Oldani, B. Rodriguez-Hernandez, L. Alfonso-Hernandez, J. F. Galindo, V. D. Kleiman, S. Fernandez-Alberti, A. E. Roitberg, S. Tretiak, Nature Comm., 9, 2316 (2018).*
8. *"Modeling fast electron dynamics with real-time time-dependent density functional theory: application to small molecules and chromophores", K. Lopata, N. Govind, Journal of Chemical Theory and Computation*, *7*(5), pp.1344-1355 (2011)
9. *"Linear-response and real-time time-dependent density functional theory studies of core-level near-edge x-ray absorption" K. Lopata, B. E. Van Kuiken, M. Khalil, N. Govind, 2012. Journal of Chemical Theory and Computation, 8(9), pp.3284-3292 (2012)*
10. "*X-ray circular dichroism signals: a unique probe of local molecular chirality", Y. Zhang, J. R. Rouxel, J. Autschbach, N. Govind, S. Mukamel, Chemical Science, 8(9), 5969 (2017)*