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Education & Professional Preparation

<i>Institution</i>	<i>Major/Area of study</i>	<i>Degree/Position, Dates</i>
Albion College	Chemistry	B.A., 1999
University of California, Berkeley	Chemistry	Ph.D., 2004
University of California, Los Angeles	Chemistry	Postdoctoral, 2005-2010

Appointments & Professional Positions

July 2010-present	Assistant Professor, Department of Chemistry, Johns Hopkins University
March-June 2010	Temporary Lecturer, Department of Chemistry & Biochemistry, UCLA

Awards & Fellowships

- The Chancellor's Award for Postdoctoral Research, UCLA, 2010
- The Amgen Award for Postdoctoral Research, Molecular Biology Institute/Department of Chemistry & Biochemistry, UCLA, 2010
- Postdoctoral Research Excellence Award, Molecular Biology Institute/Department of Chemistry & Biochemistry, UCLA, 2010
- Excellence in Postdoctoral Research, American Chemical Society, Division of Physical Chemistry, 2009
- National Science Foundation Graduate Research Fellowship, 1999-2002
- Barry M. Goldwater Scholarship, 1997-1999

Research Experience

Assistant Professor – Department of Chemistry, JHU

Research synopsis: Poly-conjugated moieties are common building blocks in molecular-based materials and electronics. Consequently, the initial ultrafast relaxation behaviors of these systems dictate the course of subsequent energy and electron transfer that underscore greater material properties and should be well-understood for efforts to improve or optimize material design and preparation methods. To this end, my group and I are investigating the ultrafast electronic and nuclear excited-state behaviors of conjugated molecules and polymers using a combination of time-resolved spectroscopies. In one research direction we are exploring non-adiabatic dynamics associated with photo-cyclic ring closure in small poly-conjugated molecules. These reactions are central to photochemical synthetic routes for creating graphene-like 2D networks of fused aromatic rings (i.e., Mallory synthesis). Understanding how intra- and intermolecular interactions dictate energy-transfer mechanisms in these systems is relevant for establishing photophysical design considerations for synthesizing new conjugated/conducting materials, and also provides fundamental insight into the coupling of electronic and vibrational states in large molecular systems (i.e., conical intersections). In a separate effort we are using time-resolved Raman spectroscopy to investigate the structural properties and dynamics of localized states on conjugated polymers commonly used in novel photovoltaic materials (e.g., poly-(3-hexylthiophene)). The goal of this work is to better understand the molecular-level characteristics of excited, charged and charge-separated intermediates in π -conjugated systems, with particular attention to how structural conformations and deformations define the spatial extent of these states along an extended 1D polymer network. Through both research efforts we are further extending the application of time-resolved, spectroscopically selective probes for interrogating molecular relaxation and reaction dynamics.

Postdoctoral – Department of Chemistry & Biochemistry, UCLA

Sponsor/Advisor: Professor Benjamin J. Schwartz

Research synopsis: Solvation is a ubiquitous process that directly influences the chemical identity and reactivity of atoms and molecules in solution. In postdoctoral work I examined the details of non-equilibrium solvation that accompanies changes in solute size and charge distribution following electron detachment and attachment in solution. Using femtosecond time-resolved spectroscopies I sought to assess how solvation is mediated by both liquid/solution structure and dynamics. In the course of my work I examined competitive electron-trapping processes in non-ideal solution environments that involve strong interactions with counterions and cosolvents (ion-pairing and preferential solvation, respectively). Furthermore, I used the solvation dynamics of atomic solutes to directly examine the applicability of linear response – the theoretical link between equilibrium and non-equilibrium relaxation behavior. In later work I was able to compare non-equilibrium solvation dynamics directly with equilibrium solute-solvent fluctuations. The latter were interrogated using three-pulse “pump-repump-probe” experiments, and it was possible to experimentally determine the dynamic solvation coordinate for a solvating atom in bulk solution resolved at the level of individual solvent molecules.

Graduate – Department of Chemistry, UC Berkeley

Advisor: Professor Daniel M. Neumark

Dissertation title: “Excited-state dynamics of molecular and cluster anions studied with time-resolved photoelectron spectroscopy and imaging”

Research synopsis: Anionic atomic and molecular clusters are experimentally tractable finite-sized chemical systems that can be used to explore the molecular-level details of fundamental dynamical behaviors, how these behaviors develop with cluster size, and how they compare to analogous processes in bulk systems. In my graduate work I interrogated the relaxation dynamics of these clusters experimentally using femtosecond time-resolved pump-probe photodetachment spectroscopy and photoelectron imaging. Specific phenomena I characterized and described in my dissertation work include: electronic relaxation mechanisms that underlie the efficient thermionic emission of carbon cluster anions; the intra-conduction-band electronic relaxation of size-selected anionic mercury clusters; and the relaxation dynamics of electronically excited anionic clusters of water. With respect to this last set of systems, my work identified additional classes of cluster isomers of relatively large size (>20 water molecules), two of which exhibit very different electronic relaxation behaviors. This work further revealed that the excited-state lifetime for the most strongly bound isomer extrapolates with cluster size towards a fast (<100-fs) relaxation for the excited excess electron in bulk water, a key species involved in radiation-induced chemistry of aqueous systems.

Representative Publications

- [1] Yu W, Zhou J, Bragg AE. Exciton conformational dynamics of poly(3-hexylthiophene) (P3HT) in solution from time-resolved resonant-Raman spectroscopy. *J. Phys. Chem. Lett.* 2012 **3**: 1321-1328.
- [2] Bragg AE, Kanu GU, Schwartz BJ. Nanometer-scale phase separation and preferential solvation in THF-water mixtures: Ultrafast electron hydration and recombination dynamics following CTTS excitation of I⁻. *J. Phys. Chem. Lett.* 2011, **2**: 2797-2804.
- [3] Bragg AE, Glover WJ, Schwartz BJ. Watching the solvation of atoms in liquids one solvent molecule at a time. *Phys. Rev. Lett.* 2010 **104**: 233005 (1-4).
- [4] Bragg AE, Cavanagh MC, Schwartz BJ. Linear response breakdown in the solvation dynamics induced by atomic electron-transfer reactions. *Science* 2008 **321**:1817-1822.
- [5] Bragg AE, Schwartz BJ. Ultrafast charge-transfer-to-solvent dynamics of iodide in tetrahydrofuran. 2. Photoinduced electron transfer to counterions in solution. *J. Phys. Chem. A* 2008 **112**: 3530-3543.
- [6] Bragg AE, Schwartz BJ. The ultrafast charge-transfer-to-solvent dynamics of iodide in tetrahydrofuran. 1. Exploring the roles of solvent and solute on electronic structure in condensed-phase charge-transfer reactions. *J. Phys. Chem. B* 2008 **112**: 483-494.

- [7] Bragg AE, Verlet JRR, Kammrath A, Cheshnovsky O, Neumark DM. Electronic relaxation dynamics of water-cluster anions. *J. Am. Chem. Soc.* 2005 **127**: 15283-15295.
- [8] Verlet JRR, Bragg AE, Kammrath A, Cheshnovsky O, Neumark DM. Observation of large water-cluster anions with surface-bound excess electrons. *Science* 2005 **307**: 93-96.
- [9] Bragg AE, Verlet JRR, Kammrath A, Cheshnovsky O, Neumark DM. Hydrated electron dynamics: From clusters to bulk. *Science* 2004 **306**: 669-671.
- [10] Stolow A, Bragg AE, Neumark DM. Femtosecond time-resolved photoelectron spectroscopy. *Chem. Rev.* 2004 **104**: 1719-1757.

External funding

Current:

American Chemical Society Petroleum Research Fund, Doctoral New Investigator Grant (ACS-PRF DNI). Project title: "Non-adiabatic Dynamics of Small Polyphenyls Studied with Time-Resolved Spectroscopies."

Submitted & Pending:

National Science Foundation, Division of Chemistry. Project title: "Conformational Order and Dynamics in Photoexcited Conjugated Polymers Revealed with Time-resolved Resonant-Raman and Absorption Spectroscopies."

Graduate students/thesis advisees

Ms. Molly Smith; B. S. in Chemistry, University of Notre Dame, 2010
 Mr. Wenjian Yu; B. Sc. in Applied Chemistry, Fudan University, 2010
 Mr. Jiawang Zhou; B. S. in Chemistry, University of Science and Technology of China, 2010
 Mr. Timothy Magnanelli; B. S. in Chemistry, UMBC, 2011
 Mr. Joshua Snyder; B. S. in Chemistry, Shippensburg University, 2011

Teaching

Fall 2011-12: Physical Chemistry Laboratory I (Chemistry 305).
 Fall 2010-12: Time-resolved Methods in Spectroscopy (Chemistry 393).
 Spring 2010: Quantum Mechanics for Chemists, Chemistry 113A (UCLA).

Synergistic activities

1. The PI has developed a graduate course on time-dependent spectroscopy which serves to: (1) familiarize graduate students and advanced undergraduates with a modern time-dependent perspective on spectroscopy, thus allowing them to understand non-linear and coherent methods; (2) introduce students with varied research interests to spectroscopic techniques now commonly used to interrogate chemical systems and materials, and (3) provide students joining the PI's research laboratory with a background knowledge of time-dependent spectroscopy. This course is appropriate for students who have taken a junior-level physical chemistry course. The lecture notes the PI has developed for this class fill the void between conventional and highly advanced spectroscopy texts, and may be developed into a short text at a later time.
2. The PI is currently adapting a physical chemistry laboratory course to have increased emphasis on scientific writing and communication. As of the fall semester of 2012, this is the only course in the department's curriculum that satisfies university writing requirements for graduation. Attention to scientific writing methods adds to discussion on formal quantitative analysis and

presentation of experimental data, experimental apparatus/instrumentation, and concepts of physical chemistry. This course has a strong impact on the scientific preparation of department majors *and* graduate teaching assistants, as TAs are usually in their first or second year of our graduate program and assist with running lab instrumentation and grading assignments.

3. Ultrafast laser laboratories and instrumentation are atypical at most universities, providing unique educational and outreach opportunities. In addition to research activity, the PI uses the lab for teaching/educational purposes, such as: demonstrations for courses (e.g., in the time-dependent spectroscopy course described above), and to introduce undergraduates and faculty from nearby institutes to ultrafast science through laboratory tours.
4. The PI continues to develop outreach activities focused on rudimentary concepts in spectroscopy – such as demonstrations and activities illustrating basic principles of light (e.g. diffraction), as well as the link between light absorption and color. The PI recently established an outreach relationship for these activities at a local (Baltimore area) elementary school (Featherbed Elementary, Woodlawn, MD), and aims to use these types of outreach programs to familiarize young students and non-scientists with important aspects of his research and its broader societal and technological impact.