

Michael J. Bedard-Hearn

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Education

- Ph.D.** Chemistry **University of California, Los Angeles, Los Angeles, CA** 2000 — 2006
Physical chemistry dissertation award (2006)
Thesis title: Understanding classical and quantum solvation dynamics in the weakly polar solvent tetrahydrofuran (THF) using projections of molecular motions in molecular dynamics simulations
Thesis advisor: Benjamin J. Schwartz
- B.S.** Chemistry **Santa Clara University, Santa Clara, CA** 1996 — 2000
3.7 gpa
American Institute of Chemists Foundation Award

Professional Experience

- Post Doctoral Fellow** *University of Texas, Austin* 2007 — Present
Dr. Peter J. Rossky Research Group
Ground and excited state quantum dynamics simulations of conjugated polymers
- Research Assistant** *University of California, Los Angeles* 2001 — 2006
Dr. Benjamin J. Schwartz Research Group
Chemistry and physics of condensed phase chemical reactions via mixed quantum/classical molecular dynamics simulations
- Teaching Assistant** *University of California, Los Angeles* 2000 — 2005
Undergraduate Courses Taught: General Chemistry I & II; Thermodynamics; Statistical Mechanics
Graduate Courses Taught: Statistical Mechanics I & II
- Research Assistant** *University of California, Los Angeles* 2000 — 2001
Dr. Jeff I. Zink Research Group
Spectroscopy of organometallic compounds
- Substitute Teacher** *San Jose (CA) Unified School District* 2000
High School Classes Taught: Physics; Chemistry; Pre-Calculus; Algebra; others
- Research Assistant** *Santa Clara University* 1999 — 2000
Dr. W. Atom Yee Research Group
Photochemistry of diphenyl butadiene
- Lab Assistant** *Santa Clara University* 1999
Summer school assistant for organic chemistry I, II, & III
- Research Assistant** *Santa Clara University* 1997 — 1999
Dr. John D. Thoburn Research Group
Double-secondary kinetic isotope effects studied with ¹H-NMR

Selected Honors/Awards

Physical Chemistry Dissertation Award

For outstanding dissertation in the field of physical chemistry, from the UCLA Department of Chemistry and Biochemistry (2006)

John Stauffer Fellowship

For excellence in research, from the UCLA Department of Chemistry and Biochemistry (2005)

Graduate Student Research Fellowship

For continuing graduate research, from the UCLA Graduate Division (2003–04)

American Institute of Chemists Foundation Award For outstanding leadership, ability, character, & scholastic achievement, Santa Clara University (2000)

Publications

8. F. Sterpone, M. J. Bedard-Hearn, & P. J. Rossky “Ground and Excited State Mixed Quantum/Classical Molecular Dynamics Simulations of π -Stacked PPV Oligomers,” in preparation June 2008.
7. M. J. Bedard-Hearn, R. E. Larsen, & B. J. Schwartz “Moving Electrons with Light: Nonadiabatic Mixed Quantum/Classical Molecular Dynamics Simulations of Relocalization of the Photoexcited Solvated Electron in Tetrahydrofuran (THF),” *J. Chem. Phys.* **125**(19), 194509 (2006).
6. R. E. Larsen, M. J. Bedard-Hearn, & B. J. Schwartz “Exploring the Role of Decoherence in Condensed-Phase Nonadiabatic Dynamics: A Comparison of Different Mixed Quantum/Classical Simulation Algorithms for the Excited Hydrated Electron,” *J. Phys. Chem. B* **110**(40), 20055 (2006).
5. M. J. Bedard-Hearn, R. E. Larsen & B. J. Schwartz, “Projections of Quantum Observables onto Solvent Degrees of Freedom in Mixed Quantum Classical Molecular Dynamics Calculations,” *Phys. Rev. Lett.* **97**, 130403 (2006).
4. M. J. Bedard-Hearn, R. E. Larsen & B. J. Schwartz, “Mean-Field Dynamics with Stochastic Decoherence (MF-SD): A New Algorithm for Nonadiabatic Mixed Quantum/Classical Molecular Dynamics Simulations with Nuclear-Induced Decoherence,” *J. Chem. Phys.* **123**, 234106 (2006).
3. M. J. Bedard-Hearn, R. E. Larsen & B. J. Schwartz “The Role of Solvent Structure in the Absorption Spectrum of Solvated Electrons: Mixed Quantum/Classical Simulations in Tetrahydrofuran(THF),” *J. Chem. Phys.* **122**, 134506 (2005).
2. M. J. Bedard-Hearn, R. E. Larsen & B. J. Schwartz “Understanding Nonequilibrium Solvent Motions Through Molecular Projections: Computer Simulations of Solvation Dynamics in Liquid Tetrahydrofuran (THF)” *J. Phys. Chem. B* **107**(51), 14464 (2003).
1. M. J. Bedard-Hearn, R. E. Larsen & B. J. Schwartz “Hidden Breakdown of Linear Response: Projections of Molecular Motions in Non-Equilibrium Simulations of Solvation Dynamics” *J. Phys. Chem. A* **107**(24), 4773 (2003).

Scientific Presentations

4. “Excited state simulations of conjugated polymers in the presence of an external electric field,” as a poster at the *American Conference on Theoretical Chemistry*, Northwestern University, Evanston, IL, July 2008.
3. “Mean-Field Molecular Dynamics with Stochastic Decoherence (MF-SD),” as a poster at the *American Conference on Theoretical Chemistry*, Los Angeles, CA, July 2005, as a poster and as one of four talks chosen from the posters at the *Gordon Research Conference: The Chemistry and Physics of Liquids*, Plymouth, NH, July 2005.
2. “The Role of Solvent Structure in the Absorption Spectrum of THF-Solvated Electrons,” as a poster at the *Western Spectroscopy Association, 52nd Annual Meeting*, Monterrey, CA, February 2005.

1. "On the Incromulence of Linear Response," as a poster at the *American Chemical Society, National Meeting*, New Orleans, LA, March 2003.

Programming Skills

FORTRAN, LaTeX, C/C++ (limited), bash/tcsh, Perl, cgi.

References

Available Upon Request