

Aaron M Virshup

Education

- 2009 **Ph.D., Physics**, *University of Illinois at Urbana-Champaign*.
Advisor: Dr. Todd Martínez
Dissertation: *First Principles Dynamics and Coarse-grained Characterization of Photoisomerization in Complex Environments*
- 2004 **M.S., Physics**, *University of Illinois at Urbana-Champaign*.
- 2003 **B.A., Physics**, *Grinnell College, Grinnell, IA*.

Research experience

- ongoing **Beratan and Yang Groups**, *Department of Chemistry, Duke University*.
- 2004–2009 **Martínez Group**, *Department of Chemistry, University of Illinois at Urbana-Champaign*.
Advisor: Dr. Todd Martínez
Investigated environmental effects on *cis-trans* photoisomerization dynamics.
Applied clustering and manifold learning techniques to build reduced-dimensional models of ultra-fast reaction paths and conical intersection seams.
Overhauled *ab initio multiple spawning* (AIMS) codebase to support modeling of large photochemical systems and to facilitate interoperability with other chemistry codes.
- 2002 **Fusion Energy Division**, *Oak Ridge National Laboratory*.
Advisor: Dr. John Caughman
Investigation of breakdown voltages in plasma heating antennas for fusion reactors.
- 2002 **Laser Interferometer Gravitational Wave Observatory (LIGO)**, *Hanford, WA*.
Advisor: Dr. Michael Landry
Investigation of noise and glitches in interferometer output.
- 2001 **Kieda Group**, *High Energy Astrophysics Institute, University of Utah*.
Advisor: Dr. David Kieda
Design of multiplexing pixel arrays for wide-angle gamma ray telescopes.

Publications

Peer-reviewed publications

Aaron M. Virshup, Chutintorn Punwong, Taras V Pogorelov, Beth Lindquist, Chaehyuk Ko, and Todd J. Martínez. Photodynamics in complex environments: Ab initio multiple spawning quantum mechanical/molecular mechanical dynamics. Feature article in *Journal of Physical Chemistry B*, **113**(11):3280–3291 (2009).

Mitchell Ong, Jeff Leiding, Hongli Tao, **Aaron M. Virshup**, and Todd J. Martínez. First principles dynamics and minimum energy pathways for mechanochemical ring-opening of cyclobutene. *Journal of the American Chemical Society*, in press (2009).

Aaron M. Virshup, Benjamin G. Levine, and Todd J. Martínez. Ab initio multiple spawning QM/MM study of ethylene photodynamics in electrostatic and steric environments. *Submitted (draft available)* (2009).

Chaehyuk Ko, **Aaron M. Virshup**, and Todd J. Martínez. Electrostatic control of the photoisomerization in the photoactive yellow protein chromophore: Hybrid QM/MM ab initio multiple spawning simulation. *Chemical Physics Letters*, **460**:272–277 (2008).

Benjamin G. Levine, Joshua D. Coe, **Aaron M. Virshup**, and Todd J. Martínez. Implementation of ab initio multiple spawning in the molpro quantum chemistry package. *Chemical Physics*, **347**:3–16 (2008).

Conference proceedings

David Kieda, Simon P. Swordy, Scott P. Wakely, **Aaron M. Virshup**. High resolution charge measurements of UH cosmic ray nuclei using a direct imaging Cherenkov ground-based observatory. *Proceedings of the SPIE*, **4858**:338–346 (2003).

In preparation

Aaron M. Virshup, Jiahao Chen, and Todd J. Martínez. Topological characterization of conical intersection seams using manifold learning techniques. *In preparation (draft available)*.

Aaron M. Virshup, Chaehyuk Ko, and Todd J. Martínez. Solvated photodynamics of the photoactive yellow protein chromophore: A hybrid QM/MM ab initio multiple spawning study. *In preparation*.

Fellowships, scholarships and awards

- 2004-2006 **Molecular Biophysics Training Grant**, *NIH and University of Illinois at Urbana-Champaign*.
- 2004 **List of teachers rated as "Excellent" by their students**, *University of Illinois at Urbana-Champaign*.
Physics 113 and Physics 114
- 2003-2004 **Graduate Assistance in Areas of National Need (GAANN) Fellowship**, *University of Illinois at Urbana-Champaign*.
- 2003 **Excellence in Physics Scholarship**, *University of Illinois at Urbana-Champaign*.
- 2002 **Energy Research Undergraduate Laboratory Fellowship**, *Department of Energy*.
- 2002 **Summer Undergraduate Research Fellowship**, *California Institute of Technology*.
- 1999-2003 **National Merit Scholarship**, *Grinnell College*.

Presentations

Talks

- 2009 **Topology of ultrafast non-adiabatic reaction paths**, *American Chemical Society 2009 March Meeting*, Salt Lake City, UT.
- 2008 **Directing photodynamics with local environment: QM/MM multiple spawning dynamics study**, *Molecular Biophysics Training Grant Meeting*, University of Illinois at Urbana-Champaign.
- 2007 **Photoisomerization selectivity in conjugated π -bond systems through local microenvironment**, *American Physical Society March Meeting*, Denver, CO.
- 2006 **Quantum Biology: First Principles Studies of Biological Photoisomerization**, *Physics Graduate Student Association Colloquium*, University of Illinois at Urbana-Champaign.

Posters

- 2008 **Reduced Dimensional Representations of Ab Initio Multiple Spawning Dynamics**, *CCP6 2008 Workshop*, University of Leeds.
- 2008 **Solvated Photodynamics of the Photoactive Yellow Protein Chromophore**, *Poster at American Conference on Theoretical Chemistry*, Northwestern University.
- 2008 **Clustering and Markov Models for Visualization and Analysis of Ultra-fast Dynamics**, *Gordon Research Conference: Atomic and Molecular Interactions*, Colby-Sawyer College.
- 2005 **Hybrid ab initio QM/MM Quantum Dynamics**, *18th Annual CMB/MB Training Grant Symposium*, University of Illinois at Urbana-Champaign.

Teaching and mentoring

- 2007 **Private tutor**, University of Illinois at Urbana-Champaign.
One-on-one mentoring for graduate-level quantum mechanics
- 2004 **Teaching Assistant**, *Introductory physics (Thermodynamics / wave mechanics)*, University of Illinois at Urbana-Champaign.
Instructor for 4 lab sections each quarter
- 2003 **Teaching Assistant**, *Introductory physics (mechanics)*, Grinnell College.
Assistant in combined lecture/lab mechanics course

Professional memberships

- American Association for the Advancement of Science
- American Chemical Society
- American Physical Society
- Royal Society of Chemistry

Technical proficiencies

Programming	Fortran 95, Perl, C, Unix shell scripting
Modeling	Amber, FMS90, Gamess-US, PC Gamess, MolPro, Mopac, Tinker
Visualization	VMD, Molekel, Molden, Avogadro, ChemDraw
Math packages	Mathematica, Maple, MatLab
Graphing/Analysis	GnuPlot, Aabel, Sigmaplot, Origin, Kaleidagraph
Presentation	iWork, MS Office, LaTeX, EndNote, Papers
Environments	Workstation Linux (Red Hat, Fedora), Cluster Linux (Rocks), Mac OS X

Summer schools / other conferences attended

- 2008 **Faraday Discussion 141: Water - From Interfaces to the Bulk**, *Heriot-Watt University, Edinburgh, UK.*
- 2006 **Summer School on Computation Materials Science: Ab Initio Molecular Dynamics Simulation Methods in Chemistry**, *University of Illinois at Urbana-Champaign.*
- 2006 **Grid Computing Workshop**, *University of Texas, Brownsville, South Padre Island, TX.*

Service

- 2006-2007 **Officer-at-large**, *University of Illinois at Urbana-Champaign Graduate Employees Organization (UIGEO).*
Elected to UIGEO's executive committee responsible for overseeing all aspects of UIGEO's mission.
- 2006 **UIGEO Delegate to Illinois Federation of Teachers Convention**, *Chicago, IL.*
Elected position.
- 2005-2006 **Bargaining committee member**, *UIGEO.*
Drafted platform to address issues in graduate work environments.
- 2003-2008 **Volunteer**, *Common Ground Food Cooperative, Urbana, IL.*
- 2003-2004 **Board of Directors**, *Community of Urbana-Champaign Cooperative Housing.*
Elected position.