Bradley F. Habenicht

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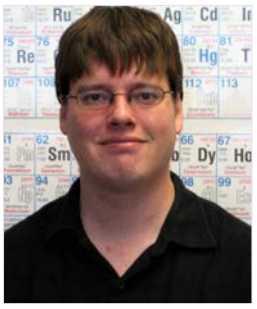

Education

Virginia Polytechnic Inst. & State University	Chemistry	B.S., 2002
University of Washington, Seattle	Theoretical Chemistry	Ph.D., 2008

Research Synopsis

- Investigations of ion transport in complex systems using computational methods.
- Using computational methods to investigate catalytic reactions for renewable energy applications.
- Understanding structure/property relationships of defined size nanoclusters as novel catalysts.

Professional Experience

2011–p	Postdoctoral Research Associate, Chemical Functionality Group, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory
2009–2011	Postdoctoral Research Associate, Department of Chemical Engineering, University of Tennessee-Knoxville
2006	Graduate Teaching Assistant (Quantum Mechanics), Department of Chemistry, University of Washington, Seattle
2005–2008	Systems Administrator, Theory Division, Department of Chemistry, University of Washington, Seattle
2004–2005	Lead Teaching Assistant (General Chemistry), Department of Chemistry, University of Washington, Seattle
2003–2004	Graduate Teaching Assistant (General Chemistry), Department of Chemistry, University of Washington, Seattle
2001–2003	Research Assistant, Organic Chemistry, Virginia Tech
2001	Research Intern, DuPont, Waynesboro, Virginia

Professional and Synergistic Activities

2011–p	Member, Materials Research Society
2010–p	Journal Reviewer, *ACS Nano, Journal of Physical Chemistry*

Honors and Awards

2007	IGERT Fellowship, University of Washington
2003	George and Agnes Irene Hoving Cady Graduate Fellowship Award, University of Washington
2003	Merck Index Award, Virginia Tech
2003	NSF Summer Undergraduate Research Program Award
1999	Marshall J. Hahn Engineering Scholarship, Virginia Tech

Invited and Contributed Conference Presentations

"Overview of Theory, Modeling, and Simulations for Optoelectronics," 4th Workshop on Sustainable Energy Future: Nanomaterials-Enabled Photovoltaics, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, TN, Sept. 19-23, 2011.

"Ab Initio Studies of the Effect of Hydrophobic Environment on Proton Transfer in Model Perfluorosulfonic Acid Systems," Solid State Proton Conductors 15 Conference, Santa Barbara, CA, Aug. 15-19, 2010.

"On the Mechanism of Proton Transport in Perfluorosulfonic Acid Systems of High Acid Density: *Ab Initio* Molecular Dynamics Simulations," South Eastern Theoretical Chemistry Association, Durham, NC, May 15-16, 2009.

"Time-Domain *Ab Initio* Studies of Excitation dynamics in Carbon Nanotubes," Non-Equilibrium Phenomena, Nonadiabatic Dynamics and Spectroscopy, Telluride, CO, Jul. 23-27, 2007.

"Electron Relaxation Dynamics in Carbon Nanotubes," American Conference on Theoretical Chemistry (ACTC05), Los Angeles, CA, Jul. 16-21, 2005.

Publications (19 Publications in Refereed Journals, 1 Book, 1 Book Chapter) *Full List Follows CV*

Graduate and Postdoctoral Advisors:

Postdoctoral Advisors:	Dr. Stephen J. Paddison (Univ. of Tennessee-Knoxville)
	Dr. Ye Xu (Oak Ridge National Laboratory)
Ph.D. Advisor:	Dr. Oleg. V. Prezhdo (Univ. of Washington; Univ. of Rochester, New York, *current)*

PUBLICATIONS

Bradley F. Habenicht, Ph.D.
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Book/Book Chapters

S. V. Kilina, B. F. Habenicht, *Excitonic and Vibrational Dynamics in Nanotechnology - Quantum Dots vs. Nanotubes*, Pan Stanford Publishing: Singapore (2009).

O. V. Prezhdo, W. R. Duncan, C. F. Craig, S. V. Kilina, B. F. Habenicht, "Photoexcitation Dynamics on the Nanoscale," Chapter 1 in *Quantum Dynamics of Complex Molecular Systems*, Springer-Verlag: Heidelberg, New York (2006).

Peer-Reviewed Publications

S. A. Fischer, B. F. Habenicht, A. B. Madrid, W. R. Duncan, O. V. Prezhdo, "Regarding the Validity of the Time-Dependent Kohn-Sham Approach for Electron-Nuclear Dynamics via Trajectory Surface Hopping," *Journal of Chemical Physics* **134**(2), 024102-024111 (2011).

B. F. Habenicht, S. J. Paddison, M. E. Tuckerman, "*Ab Initio* Molecular Dynamics Simulations Investigating Proton Transfer in Perfluorosulfonic Acid Functionalized Carbon Nanotubes," *Physical Chemistry Chemical Physics* **12**, 8728-8732 (2010).

B. F. Habenicht, S. J. Paddison, M. E. Tuckerman, "The Effects of the Hydrophobic Environment on Proton Mobility in Perfluorosulfonic Acid Systems: An *Ab Initio* Molecular Dynamics Study," *Journal of Materials Chemistry* **20**, 6342-6351 (2010).

V. V. Chaban, O. N. Kalugin, B. F. Habenicht, O. V. Prezhdo, "The Influence of the Rigidity of a Carbon Nanotube on the Structure and Dynamics of Confined Methanol," *Journal of Physical Society Japan* **79**, 064608-064612 (2010).

Z. Guo, B. F. Habenicht, W.-Z. Liang, O. V. Prezhdo, "*Ab Initio* Study of Phonon-Induced Dephasing of Plasmon Excitations in Silver Quantum Dots," *Physical Review B* **81**, 125415-125420 (2010).

A. B. Madrid, K. Hyeon-Deuk, B. F. Habenicht, O. V. Prezhdo, "Phonon-Induced Dephasing of Excitons in Semiconductor Quantum Dots: Multiple Exciton Generation, Fission, and Luminescence," *ACS Nano* **3**(9), 2487-2494 (2009).

B. F. Habenicht and O. V. Prezhdo, "Time-Domain *Ab Initio* Study of Nonradiative Decay in a Narrow Graphene Ribbon," *The Journal of Physical Chemistry C* **113**(32), 14067-14070 (2009).

H. Bao, B. F. Habenicht, O. V. Prezhdo, X. Ruan, "Temperature Dependence of Hot-Carrier Relaxation in PbSe Nanocrystals: An *Ab Initio* Study," Physical Review B **79**(23), 235306-235313 (2009).

B. F. Habenicht, O. N. Kalugin, O. V. Prezhdo, "*Ab Initio* Study of Phonon-Induced Dephasing of Electronic Excitations in Narrow Graphene Nanoribbons," *NANO Letters* **8**(8), 2510-2516 (2008).

B. F. Habenicht, S. V. Kilina, O. V. Prezhdo, "Comparative Analysis of Electron-Phonon Relaxation in a Semiconducting Carbon Nanotube and a PbSe Quantum Dot," *Pure Applied Chemistry* **80**(7), 1433-1448 (2008).

B. F. Habenicht and O. V. Prezhdo, "Nonradiative Quenching of Fluorescence in a Semiconducting Carbon Nanotube: A Time-Domain *Ab Initio* Study," Physical Review Letters **100**(19), 197402-197405 (2008).

B. F. Habenicht and O. V. Prezhdo, "Nanotube Devices: Watching Electrons in Real Time," *Nature Nanotechnology* **3**, 190-191 (2008).

B. F. Habenicht, H. Kamisaka, K. Yamashita, O. V. Prezhdo, "*Ab Initio* Study of Vibrational Dephasing of Electronic Excitations in Semiconducting Nanotubes," *NANO Letters* **7**(11), 3260-3265 (2007).

B. F. Habenicht, C. F. Craig, O. V. Prezhdo, "Time-Domain *Ab Initio S*imulation of Electron and Hole Relaxation Dynamics in a Single-Wall Semiconducting Carbon Nanotube," *Physical Review Letters* **96**(18), 187401-187404 (2006).

H. W. Gibson, H. Wang, K. Bonrad, J. W. Jones, C. Slebnodnick, P. Lobue, "Regioselective Routes to Disubstituted Dibenzo Crown Ethers and Their Complexations," *Organic and Biomolecular Chemistry* **3**(11), 2114-2121 (2005).