

Matthew G. Reuter

Education

- Sep. 2006 – **Doctor of Philosophy (Ph.D.)**, *Northwestern University*, Evanston, IL.
Jun. 2011 Dissertation Title: *Coherent Control of Electric Current at the Nanoscale*
Field: Chemistry
Thesis Advisers: Professors Mark A. Ratner and Tamar Seideman
U.S. Department of Energy Computational Science Graduate Fellow (DOE CSGF), Sep. 2007 – Jun. 2011
- Aug. 2002 – **Bachelor of Science (B.Sc.)**, *Michigan Technological University*, Houghton, MI.
Apr. 2006 Majors: Chemistry, Mathematics, Cheminformatics, Bioinformatics
Minor: Computer Science
Summa Cum Laude, GPA: 4.0/4.0

Professional Experience

- Jan. 2015 – **Assistant Professor**, *Institute for Advanced Computational Science and Department of Applied Mathematics & Statistics, Stony Brook University*, Stony Brook, NY.
Present
- Oct. 2013 – **Research Associate**, *Department of Chemistry, Northwestern University*, Evanston, IL.
Dec. 2014 **Postdoctoral Fellow**, Oct. 2013 – Feb. 2014
• Developing models to understand single molecule experiments (working closely with the experimental group of Prof. Richard Van Duyne) • Elucidating the information content of conductance histograms • Investigating destructive interference effects in electron transport.
- Aug. 2011 – **Research Scientist**, *Computer Science and Mathematics Division and Center for Nanophase Materials Sciences, Oak Ridge National Laboratory*, Oak Ridge, TN.
Oct. 2013 **Eugene P. Wigner Fellow**, Aug. 2011 – Aug. 2013
• Developing methods to model finite, elongated nanomaterials with defects • Deriving theories for understanding experimental electron transport data (conductance histograms) • Using projection operators to reconsider electron transport theories • Investigating the complex band structure of materials • Exploring the properties and applications of matrix Möbius transformations.

Research Interests

Surface Effects, Defects, & Disorder in Materials

- Investigating the decay lengths of surface effects in materials of different dimensionality
- Calculating the effects of disorder in these systems
- Developing efficient algorithms for such studies
- Formulating complex band structure and developing its applications.

Electric Current through Nanoscale Transport Junctions

- Understanding the information content of experimental conductance histograms
- Quantifying cooperative (multi-channel) effects in transport junctions
- Developing more accurate and more efficient computational techniques for electron transport; specifically, exorcising ghost transmission.

Recent Collaborators

- Robert J. Harrison (Stony Brook University)
- Herre van der Zant (Delft University of Technology)
- Latha Venkataraman (Columbia University)
- Emily A. Weiss (Northwestern University)
- Gemma C. Solomon (University of Copenhagen)
- Thorsten Hansen (University of Copenhagen)
- Ferdinand C. Grozema (Delft University of Technology)
- Judith C. Hill (Oak Ridge National Laboratory).

Funding Record

- Aug. 2011 – **Eugene P. Wigner Fellowship**, *An Accurate and Efficient Computational Methodology for Simulating Disordered Nanoscale Materials: Toward the Rational Design of Better Batteries.*
Aug. 2013 **M. G. Reuter** (P.I.), B. G. Sumpter (mentor); \$468,600.
- Sep. 2007 – **U.S. Department of Energy Computational Science Graduate Fellowship.**
Jun. 2011 **M. G. Reuter** (P.I.), M. A. Ratner (adviser), T. Seideman (adviser); \$350,000 (estimated).

Publications

Peer-Reviewed Journals

- () R. J. Harrison, G. Beylkin, J. Calvin, G. I. Fann, J. Fosso-Tande, D. A. Galindo, J. R. Hammond, R. J. Hartman-Baker, J. C. Hill, J. Jia, B. J. Mintz, **M. G. Reuter**, N. A. Romero, H. Sekino, V. Slavici, K. Stock, P. M. Sutter, W. S. Thornton, E. Valeev, Á. Vázquez-Mayagoitia, N. E. Vence, "MADNESS: A Multiresolution, Adaptive Numerical Environment for Scientific Simulation," *In Preparation*.
- () **M. G. Reuter**, "Formulating Complex Band Structure with Wavefunctions and Green Functions," *In Preparation*.
- () **M. G. Reuter**, W. S. Thornton, B. E. Sundahl, R. J. Harrison, "Removing the Stigma of Nonorthogonal Basis Sets from Computational Quantum Mechanics: Rules for Translating Operator Expressions to their Matrix Representations," *In Preparation*.
- () G. Zhang, M. A. Ratner, **M. G. Reuter**, "Is Molecular Rectification Caused by Asymmetric Electrode Couplings or by a Molecular Bias Drop?," *J. Phys. Chem. C*, *Submitted*.
- 21. N. M. Boffi, J. C. Hill, **M. G. Reuter**, "Characterizing the Inverses of Block Tridiagonal, Block Toeplitz Matrices," *Comput. Sci. Discov.* **8**, 015001 (2015).
- 20. **M. G. Reuter**, T. Hansen, "Finding Destructive Interference Features in Molecular Transport Junctions," *J. Chem. Phys.* **141**, 181103 (2014). • **COMMUNICATION**
- 19. N. E. Jackson, H. M. Heitzer, B. M. Savoie, **M. G. Reuter**, T. J. Marks, M. A. Ratner, "Emergent Properties in Locally Ordered Molecular Materials," *Isr. J. Chem.* **54**, 454–466 (2014).
- 18. **M. G. Reuter**, R. J. Harrison, "Response to 'Comment on 'Rethinking First-Principles Electron Transport Theories with Projection Operators: The Problems Caused by Partitioning the Basis Set' [J. Chem. Phys. **140**, 177103 (2014)]," *J. Chem. Phys.* **140**, 177104 (2014).
- 17. **M. G. Reuter**, R. J. Harrison, "Rethinking First-Principles Electron Transport Theories with Projection Operators: The Problems Caused by Partitioning the Basis Set," *J. Chem. Phys.* **139**, 114104 (2013).
- 16. P. D. Williams, **M. G. Reuter**, "Level Alignments and Coupling Strengths in Conductance Histograms: The Information Content of a Single Channel Peak," *J. Phys. Chem. C* **117**, 5937–5942 (2013).
- 15. **M. G. Reuter**, N. M. Boffi, M. A. Ratner, T. Seideman, "The Role of Dimensionality in the Decay of Surface Effects," *J. Chem. Phys.* **138**, 084707 (2013).
- 14. **M. G. Reuter**, J. C. Hill, "An Efficient, Block-by-Block Algorithm for Inverting a Block Tridiagonal, Nearly Block Toeplitz Matrix," *Comput. Sci. Discov.* **5**, 014009 (2012).
- 13. **M. G. Reuter**, M. A. Ratner, T. Seideman, "Laser Alignment as a Route to Ultrafast Control of Electron Transport through Junctions," *Phys. Rev. A* **86**, 013426 (2012).
- 12. **M. G. Reuter**, M. C. Hersam, T. Seideman, M. A. Ratner, "Signatures of Cooperative Effects and Transport Mechanisms in Conductance Histograms," *Nano Lett.* **12**, 2243–2248 (2012).
- 11. A. J. Morris-Cohen, V. Vasilenko, V. A. Amin, **M. G. Reuter**, E. A. Weiss, "Model for Adsorption of Ligands to Colloidal Quantum Dots with Concentration-Dependent Surface Structure," *ACS Nano* **6**, 557–565 (2012).
- 10. **M. G. Reuter**, J. C. Hill, R. J. Harrison, "Solving PDEs in Irregular Geometries with Multiresolution Methods I: Embedded Dirichlet Boundary Conditions," *Comput. Phys. Commun.* **183**, 1–7 (2012).
- 9. **M. G. Reuter**, T. Seideman, M. A. Ratner, "Molecular Conduction through Adlayers: Cooperative Effects Can Help or Hamper Electron Transport," *Nano Lett.* **11**, 4693–4696 (2011).
- 8. **M. G. Reuter**, G. C. Solomon, T. Hansen, T. Seideman, M. A. Ratner, "Understanding and Controlling Crosstalk Between Parallel Molecular Wires," *J. Phys. Chem. Lett.* **2**, 1667–1671 (2011).
- 7. **M. G. Reuter**, T. Seideman, M. A. Ratner, "Guidelines for Choosing Molecular 'Alligator Clip' Binding Motifs in Electron Transport Devices," *J. Chem. Phys.* **134**, 154708 (2011).
- 6. **M. G. Reuter**, T. Seideman, M. A. Ratner, "Probing the Surface-to-Bulk Transition: A Closed-Form, Constant-Scaling Algorithm for Calculating Subsurface Green Functions," *Phys. Rev. B* **83**, 085412 (2011). • **"EDITORS' SUGGESTION" ARTICLE**.

5. **M. G. Reuter**, "Closed-Form Green Functions, Surface Effects, and the Importance of Dimensionality in Tight-Binding Metals," *J. Chem. Phys.* **133**, 034703 (2010).
4. **M. G. Reuter**, M. A. Ratner, T. Seideman, "A Fast Method for Solving Both the Time-Dependent Schrödinger Equation in Angular Coordinates and its Associated 'm-mixing' Problem," *J. Chem. Phys.* **131**, 094108 (2009). • **TOP DOWNLOADS, SEP. 2009.**
3. A. M. Spokoyny, **M. G. Reuter**, C. L. Stern, M. A. Ratner, T. Seideman, C. A. Mirkin, "Carborane-Based Pincers: Synthesis and Structure Reactivity of SeBSe and SBS Pd(II) Complexes," *J. Am. Chem. Soc.* **131**, 9482–9483 (2009). • **HIGHLIGHTED IN ANGEW. CHEM. INT. ED. 49 252-255, (2010).**
2. **M. G. Reuter**, T. Hansen, T. Seideman, M. A. Ratner, "Molecular Transport Junctions with Semiconductor Electrodes: Analytical Forms for One-Dimensional Self-Energies," *J. Phys. Chem. A* **113**, 4665–4676 (2009).
1. **M. G. Reuter**, M. Sukharev, T. Seideman, "Laser Field Alignment of Organic Molecules on Semiconductor Surfaces: Toward Ultrafast Molecular Switches," *Phys. Rev. Lett.* **101**, 208303 (2008). • **HIGHLIGHTED IN NATURE PHOTON. 3, 4–5 (2009).**

Commentaries & Perspectives

1. **M. G. Reuter**, L.-W. Wang, "Quantum Mechanics without Wavefunctions," *SIAM News* **46**, vol. 5 (June 2013). • **INVITED COMMENTARY ON THE 2013 SIAM CONFERENCE ON COMPUTATIONAL SCIENCE & ENGINEERING.**

Selected Presentations

Invited Lectures

- 30 May 2014 **M. G. Reuter**, "Reconciling Experiment and Theory/Computation in Studies of Electron Transport," *Institute for Advanced Computational Science, Stony Brook University, Stony Brook, NY.*
- 15 Nov. 2013 **M. G. Reuter**, R. J. Harrison, "Exorcising Ghost Transmission from Electron Transport Calculations: Refighting Old Battles in New Contexts," *22nd Conference on Current Trends in Computational Chemistry, Jackson, MS (15 – 16 Nov. 2013).*
- 26 Jul. 2012 **M. G. Reuter**, "You Should Also Think About Complicated Things (to Improve Computation): Exorcising Numerical Ghosts from Electron Transport Calculations," *Department of Energy Computational Science Graduate Fellowship Annual Conference, Arlington, VA (26 – 28 Jul. 2012).* • **2012 FREDERICK A. HOWES SCHOLAR LECTURE.**

Contributed Lectures

- 5 Mar. 2014 **M. G. Reuter**, R. J. Harrison, "Exorcising Ghost Transmission from Electron Transport Calculations: Refighting Old Battles in New Contexts," *2014 March Meeting of the American Physical Society, Denver, CO (3 – 7 Mar. 2014).*
- 20 Mar. 2013 **M. G. Reuter**, P. D. Williams, "The Information Content of Conductance Histogram Peaks: Transport Mechanisms, Level Alignments, and Coupling Strengths," *2013 March Meeting of the American Physical Society, Baltimore, MD (18 – 22 Mar. 2013).*
- 28 Feb. 2013 **M. G. Reuter**, "Exorcising Ghost Transmission from *ab initio* Calculations of Electron Transport," *SIAM Conference on Computational Science and Engineering, Boston, MA (25 Feb. – 1 Mar. 2013).*
- 1 Mar. 2012 **M. G. Reuter**, T. Seideman, M. A. Ratner, "Understanding Crosstalk between Parallel Molecular Wires," *2012 March Meeting of the American Physical Society, Boston, MA (27 Feb. – 2 Mar. 2012).*
- 21 Jul. 2011 **M. G. Reuter**, T. Seideman, M. A. Ratner, "Computational Science Meets Materials Chemistry: A Bilingual Investigation of Surface Effects in Nanoscale Systems," *Department of Energy Computational Science Graduate Fellowship Annual Conference, Arlington, VA (21 – 23 Jul. 2011).*

Posters

- 6–7 Aug. 2014 **M. G. Reuter**, "Understanding and Interpreting Single Molecule Behavior: The Information Content of Conductance Histograms," *Gordon Research Conference on Electron Donor-Acceptor Interactions, Newport, RI (3 – 8 Aug. 2014).*

- 25 Sep. 2013 **M. G. Reuter**, B. G. Sumpter, "An Accurate and Efficient Computational Methodology for Simulating Disordered Nanoscale Materials," *2013 ORNL LDRD Poster Session*, Oak Ridge, TN. • **BEST POSTER**
- 6 Aug. 2012 **M. G. Reuter**, "Exorcising Ghost Transmission from *ab initio* Calculations of Electron Transport," *Gordon Research Conference on Electron Donor-Acceptor Interactions*, Newport, RI (5 – 10 Aug. 2012).

Teaching & Related Experience

- Jan. – **Co-Instructor**, *Integrated Science Program, Northwestern University*, Evanston, IL.
 Mar. 2014 Designed curricula, lectures, and assignments for an introductory undergraduate course on scientific computing.
- Sept. 2006 – **Teaching Assistant**, *Department of Chemistry, Northwestern University*, Evanston, IL.
 Jun. 2008 Supervised general chemistry and spectroscopy laboratories, graded examinations and laboratory reports, recited thermodynamics. Pioneered a recitation section for graduate-level quantum chemistry: lectured mathematics reviews and wrote exercise sets.
- Aug. 2005 – **Teaching Assistant**, *Department of Chemistry, Michigan Technological University*, Houghton, MI.
 Apr. 2006 Taught physical chemistry laboratories, graded laboratory reports, and contributed to the modification and improvement of experiments.
- May 2004 – **Coach/Head Coach**, *Chemistry Learning Center, Michigan Technological University*, Houghton, MI.
 Aug. 2005 Coached students in general and organic chemistry while supervising other coaches and helping administrate the learning center.
- Aug. 2001 – **Tutor**, *Writing Tutorial Center, Plymouth-Salem High School*, Canton, MI.
 Jan. 2002 Provided peer critiques of students' compositions, encouraged critical thinking, and publicized use of the center.

Mentoring Experience

- Jan. – **Christopher S. Pitler & Robert Quan**, *Northwestern University Undergraduate Students*
 Jun. 2014 Examining the influence of vacuum tunneling in conductance histograms.
- Jul. 2013 – **Gaibo Zhang**, *Oak Ridge High School Student (Math-Science Senior Thesis)*
 May 2014 Understanding the information content of voltage-dependent conductance histograms. • **1 PUBLICATION**
- Jun. – **Nicholas M. Boffi**, *Science Undergraduate Laboratory Internship (SULI) Student*
 Aug. 2013 Exploring the properties of matrix Möbius transformations and their relation to block tridiagonal, block Toeplitz matrices. • **1 PUBLICATION** • **2014-15 FULBRIGHT FELLOW** • **2014 DOE COMPUTATIONAL SCIENCE GRADUATE FELLOW (DEFERRED)**
- Jun. 2012 – **Patrick D. Williams**, *Oak Ridge High School Student (Math-Science Senior Thesis)*
 May 2013 Exploring the information contained in the line shapes of (zero-bias) conductance histogram peaks and developing methods to extract this information from experimental data. • **1 PUBLICATION** • **SEMI-FINALIST IN THE 2012 SIEMENS NATIONAL MATH AND SCIENCE COMPETITION** • **5th PLACE IN THE 2013 SOUTHERN APPALACHIAN SCIENCE AND ENGINEERING FAIR**
- Oct. 2010 – **Nicholas M. Boffi**, *Northwestern University Undergraduate Student*
 Aug. 2011 Understanding the role of dimensionality in the decay of surface effects. • **1 PUBLICATION**

Professional Service

- Reviewer**, • ACS Nano • Comput. Sci. Discov. • J. Chem. Phys. • J. Comput. Phys. • J. Phys. Chem. • J. Phys. Chem. Lett. • Nanotechnology • Nature Commun.
- Jan. – **Member**, *DOE CSGF Screening Committee*.
 Feb. 2015 Reviewed applications for the Department of Energy Computational Science Graduate Fellowship (DOE CSGF) program and made recommendations to the Selection Committee.
- Jul. 2014 **Poster Review Organizer**, *Fellows' Poster Session*, 2014 DOE CSGF Program Review, Arlington, VA.
- Nov. 2013 – **Co-Organizer**, *2014 Midwest Theoretical Chemistry Conference*, Northwestern University, Evanston, IL.
 Jun. 2014 Helped organize the conference: setting the format, inviting speakers, advertising, coordinating logistics, etc.
- Jul. 2013 **Poster Review Organizer**, *Fellows' Poster Session*, 2013 DOE CSGF Program Review, Arlington, VA.
 Apr. – **Co-Organizer**, *1st Annual ORNL Postdoc Research Symposium*, Oak Ridge National Laboratory, Oak Ridge, TN.
 Jul. 2013 Helped organize a day-long symposium for ~100 ORNL postdoctoral researchers to present their research.

- Jan. – **Member**, *DOE CSGF Screening Committee*.
- Feb. 2013 Reviewed applications for the Department of Energy Computational Science Graduate Fellowship (DOE CSGF) program and made recommendations to the Selection Committee.
- Jul. 2012 **Poster Judge**, *Fellows' Poster Competition*, 2012 DOE CSGF Annual Conference, Arlington, VA.
- Jun. – **Member**, *Graduate Student and Postdoc Planning Committee*, 2008 American Conference on Theoretical Chemistry, Evanston, IL.

Volunteer Experience & Community Engagement

- Oct. 2013 – **Member**, *Ridgeville Band of Evanston*, Evanston, IL.
- Dec. 2014 Played trombone for free concerts at nursing homes, medical centers, and at community events.
- Jan. 2014 **Judge**, *St. Athanasius School Science Fair*, Evanston, IL.
Judged and provided feedback on seventh- and eighth-grade science fair projects.
- Sep. 2011 – **Member/Assistant Conductor**, *Tennessee Valley Ensemble*, Knoxville, TN.
- Sep. 2013 Played trombone for free concerts at nursing homes, medical centers, and at various community events. Occasionally directed rehearsals and concerts.
- Nov. 2011 – **Volunteer**, *Knoxville Area Rescue Ministries*, Knoxville, TN.
- Dec. 2012 Prepared and served bimonthly meals for 150–250 impoverished people in the Knoxville area.
- Jun. – **Member**, *Team Bookin' It*, Chicago, IL.
- Sep. 2012 Raised \$850 to combat illiteracy in Chicago schools through Open Books, Ltd.; ran the 2012 Chicago half-marathon in 1:46:30.
- Sep. 2008 – **Volunteer/Team Leader**, *Hilda's Place Shelter*, Evanston, IL.
- May 2011 Planned, prepared, and served monthly meals at the Hilda's Place homeless shelter.
- Sep. 2007 – **Volunteer**, *Northwestern University/National Science Foundation Science in the Classroom Program*, Evanston/Chicago, IL.
- Feb. 2011 Helped plan, teach, and revise introductory science experiments for third- and fourth-grade students in the Chicago public schools.
- Sep. 2003 – **Assistant Coach**, *Hancock High School Science Olympiad*, Hancock, MI.
- Mar. 2004 Coached and mentored students in biological and physical sciences and the scientific method.

Honors & Awards

- Frederick A. Howes Scholar in Computational Science, U.S. Department of Energy, 2012.
- Commendation for Excellence in Graduate Research, Department of Chemistry, Northwestern University, 2011.
- Eugene P. Wigner Fellow, Oak Ridge National Laboratory, 2011 – 2013.
- Edmund W. Gelewitz Award for Excellence in Research and Service, Department of Chemistry, Northwestern University, 2010.
- Northwestern University/Weizmann Institute of Science Student Exchange Scholarship, 2009.
- Donald E. Smith Award for Excellence in Graduate-Level Teaching, Department of Chemistry, Northwestern University, 2008.
- U.S. Department of Energy Computational Science Graduate Fellow, 2007 – 2011.
- Department of Chemistry Excellence Award, Michigan Technological University, 2006.
- Department of Chemistry Outstanding Senior Award, Michigan Technological University, 2006.
- Charles Knobloch Mathematics Scholarship Award, Department of Mathematical Sciences, Michigan Technological University, 2006.
- Norman E. Scholz Award as the Outstanding Mathematics Senior, Department of Mathematical Sciences, Michigan Technological University, 2006.
- Leslie Leifer Award in Physical Chemistry, Department of Chemistry, Michigan Technological University, 2005.
- Department of Chemistry Ambassador Award, Michigan Technological University, 2004, 2005.
- The Honor Society of Phi Kappa Phi, 2004.

- The National Dean's List, 2004, 2005.
- Michigan Technological University Dean's List, FS2002 – 03, FS2003 – 04, FS2004 – 05, F2005 – 06.
- Michigan Technological University College of Sciences and Arts Dean's List, 2002 – 03, 2003 – 04, 2004 – 05.
- Michigan Technological University Board of Control Scholarship, 2002 – 2006.
- Gary Grant Hees Scholarship, Plymouth-Canton Educational Park, 2002.
- Who's Who Among American High School Students, 2000.
- Bands of America Grand National Champions with Captions for Outstanding Musical Performance and Outstanding General Effect, Plymouth-Canton Educational Park Marching Band, 1999.
- Lockheed-Martin/Wayne County RESA NASA Space Camp Scholarship, 1996.

Professional Memberships

2014 – *Present* Society for Industrial and Applied Mathematics
 2010 – *Present* American Physical Society
 2006 – *Present* American Chemical Society

Computer Skills

Operating Systems Linux (Fedora), Mac OS X (Mavericks), Windows XP
 Programming Languages C/C++, Fortran 90, Java, PHP, Python, Common Lisp, C#, Shell Scripting
 Programming Resources MADNESS, GNU Scientific Library, MPI, SQL, OpenGL
 General Software VI, L^AT_EX, MS Office Suite
 Technical Software Mathematica, Gnuplot, GAMESS, Q-Chem, NWChem

Interests

Fitness Distance Running, Jogging, Circuit Training
 Music Playing Trombone, Arranging Music for Small Ensembles, Listening to Classical/Instrumental and Classic Rock
 Culinary Baking, Cooking, Wine Tasting