Joshua A. Schrier
Associate Professor of Chemistry

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Appointments

Haverford College		Haverford, PA
	Chair	2017-present
	Associate Professor of Chemistry	2015-present
	Assistant Professor of Chemistry	2008-2015
Lawrence Berkeley National Laboratory		Berkeley, CA
	Luis W. Alvarez Postdoctoral Fellow	2005-2008

Education

University of California, Berkeley		Berkeley, CA
	Ph.D. in Chemistry	2005
St. Peter's College		Jersey City, NJ
	BS *Summa Cum Laude* in Chemistry	2000

Training

Lawrence Berkeley National Laboratory		Berkeley CA
	Postdoctoral fellow with Lin-Wang Wang	2005-2008
University of California, Berkeley		Berkeley, CA
	Graduate student with K. Birgitta Whaley	2000-2005

Awards

US Department of Energy, Visiting Faculty Program Summer 2017
Research at Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, CA

Fulbright Scholar Fall 2015
Research at Fritz Haber Institute - Max-Planck-Gesellschaft, Berlin, Germany

Henry Dreyfus Teacher-Scholar Award 2014-2019

Research Corporation for Scientific Advancement 2011-2013
Cottrell College Science Award

Kavli Institute for Theoretical Physics 2011-2013
KITP Scholar 2011-2013

Petroleum Research Foundation
Undergraduate New Investigator Award 2009-2011

Lawrence Berkeley National Laboratory
Alvarez Postdoctoral Fellowship in Computational Sciences 2005-2008

National Defense Science & Engineering Graduate (NDSEG) Fellowship 2001-2004

United States Army Research Office
Quantum Computing Graduate Research Fellow 2001-2003

University of California, Berkeley
Abramson Graduate Scholarship 2001

Barry M. Goldwater Scholar 1999

St. Peter's College 1996-2000
Full Academic Scholarship

External Grants and Contracts

National Science Foundation (DMR-1709351) 2017-2020
"CDS&E: D3SC: The Dark Reaction Project: A machine-learning approach to exploring structural diversity in solid state synthesis", awarded jointly with Prof. Sorelle Friedler (Computer Science) and Prof. Alexander Norquist (Chemistry) $645,288

National Science Foundation (CHE-1626238) Aug 2016
"MRI: Addition of High Performance Computers for the Molecular Education and Research Consortium in Undergraduate computational chemistry (MERCURY)", PIs: George C. Shields (Furman), Maria A Gomez (Mt. Holyoke), Carol A. Parish (Univ. Richmond), Marc Zimmer (Connecticut College) and 23 other collaborators, $225,000

Deutscher Akademischer Austausch Dienst (DAAD) July 2016
"Learn German in Germany" Faculty Language Training award

Camille & Henry Dreyfus Foundation (TH-14-010) 2014-2019
Henry Dreyfus Teacher-Scholar Award, $60,000

National Science Foundation (DMR-1307801) 2013-2016
"The Dark Reaction Project: A Machine Learning Approach to Materials Discovery", awarded jointly with Prof. Sorelle Friedler (Computer Science) and Prof. Alexander Norquist (Chemistry) $299,998

Research Corporation for Scientific Advancement (#20051) 2011-2013
Cottrell College Science Award, "Chemical and Isotopic Separations using Quantum Tunneling Effects" $35,000 plus $15,000 institutional matching funds.

Petroleum Research Foundation (49409-UNI10) 2009-2011
Undergraduate New Investigator Award, "Comprehensive Atomistic Modeling of Thermoelectric Semiconductor Nanowire Heterostructures," $50,000

Internal Grants

Teaching with Technology Program 2015, 2016
"A Web-based Game for Teaching Organic Spectroscopy", $6,000

Mellon Foundation Tri-College Seed Grant 2014-2016
"Philadelphia Theoretical Chemistry Club," awarded jointly with Profs. Joseph Subotnik (Univ. of Pennsylvania), Michele Francl (Bryn Mawr), and Paul Rablen (Swarthmore), $3,000

Howard Hughes Medical Institute and Teaching With Technology Program 2013-2014
"HaverFab Maker Space for the Arts and Sciences", awarded jointly with Profs. Sorelle Friedler (Computer Science), Markus Baenzinger (Fine Arts), Suzanne Amador Kane (Physics), Hank Glassman (East Asian Studies) Bruce Boyes (Machinist), George Neusch (Biology Technician), Daniel Fabry (Chemistry Technician), $24,600

Koshland Integrated Natural Sciences Center Special Faculty Projects 2012
"Enhancing Scientific Computer Infrastructure in the KINSC", awarded jointly with Prof. Beth Wilman (Astronomy) and Prof. Peter Love (Physics). $20,000 to support a UNIX support specialist.

Mellon Foundation Arts Residency Planning Grant 2009
"The Sound of Sci(l)ence: Listening to Quantum Mechanics, the Big Bang, and Nanotechnology", joint with Prof. Stephon Alexander (Physics), $10,000

Center for Peace and Global Citizenship and Koshland Natural Sciences Center 2008-2010

"The Solar Project: Integrating Solar Energy into the Campus and Curriculum", joint with Prof. Suzanne Amador Kane (Physics) and Walter Smith (Physics), $18,000

Service

-Haverford College

Chemistry Department Chair	(2017-present)
Scientific Computing Concentration Coordinator	(2010-present)
Laboratory and Biosafety Committee	(2010-11, 2012-'14, 2017-)
At-Large Representative to Alternate Academic Council	(2016-'17)
Koshland Integrated Natural Sciences Center (KINSC) Steering Committee	(2016-'17)
Library Advisory Committee, Faculty representative	(2016-'17)
Visible Curriculum Working Group	(2016-'17)
Chief Information Officer Search, Faculty co-chair	(2014-2015)
Faculty Mentor for new faculty in Japanese Department	(2014-2015)
Information Technology Policy Committee, Faculty Representative	(2013-2014)
Bryn Mawr Geochemistry Search Committee	(2010-2011)
Environmental Studies Concentration working group	(2009-2010)
Committee for Environmental Responsibility, Faculty Representative	(2009-2011)

-Reviewing (past 4 years)

Ad hoc reviewer for: *ACS Appl. Mater. Interf.; ACS Nano; Am. J. Phys.; Chemical Engineering Journal; Chemistry of Materials; Chemical Physics Letters; Computational Materials Science; Inorg. Chem.; Journal of Chemical Physics; Journal of Physical Chemistry A / B/C/Lett.; Journal of Physics D: Applied Physics; Journal of Nanoscience and Nanotechnology; Langmuir; Nature Nanotechnology; Materials Today, Physical Review A / B; Scientific Reports*

Proposal reviewer for: Royal Society (UK) (2017); National Science Foundation (USA)—Macromolecular, Supramolecular, and Nanochemistry (2017) & Chemistry, Theory, Modeling (2016); Partnership for Advanced Computing in Europe (PRACE) (2017); Irish Centre for High-End Computing Class A allocation awards (2017); ACS Petroleum Research Fund (2017-2015, 2012); Research Foundation—Flanders (FWO) (2016, 2014); U.S. DOE Office of Science Graduate Fellowship Panel Review (2012)

Study Groups:

Mission Innovation "Energy Materials Innovation Workshop" (Mexico City, 11-14 September 2017); cross-panel discussion chair "Theory"

NSF Workshop on "Framing the Role of Big Data and Modern Data Science in Chemistry" (Arlington, VA, 17-19 April 2017); Invited talk on "*What is the current state of data science to support decision making in chemical research?"*

Education Working group, NSF Workshop on "The Rise of Data in Materials Research", (University of Maryland, 29-30 June 2015)

Chemistry Study Group, Committee on the Undergraduate Program in Mathematics, Mathematical Association of America (Oct 2013-Mar 2014)

Symposium Planning:

Pacifichem 2015 "Data Mining and Machine Learning Meets Experiment and First-Principles Simulation for Materials Discovery" (2 day session), organized with Prof. Shuichi Iwata (Univ. of Tokyo, Japan), Carlos Amador-Bedolla (National Autonomous Univ. of Mexico (UNAM)), Tom Woo (Univ. of Ottowa, Canada)

American Chemical Society National Meeting, Fall 2013 "Applications of Theoretical Chemistry for Energy and Fuel Production" (Division of Energy and Fuels), organized with Dr. De-En Jiang (Oak Ridge National Laboratory) and Prof. Guofeng Wang (Univ. of Pittsburgh)

Courses Taught

Advanced General Chemistry (Chem105)—Accelerated one-semester treatment of general chemistry for students with advanced preparation. (This course is no longer offered, due to changes in the curriculum.) *Spring 2009, Spring 2010.*

Chemical Structure and Bonding (Chem111 and Chem115)—Structure and bonding in molecules starting from nuclear and electronic structure of atoms. This course introduces the theories of chemical bonding that rationalize and predict the structures and properties of molecules and materials. It also introduces modern spectroscopic and computational methods used to study chemical structure and bonding. (Freshman level course). *Fall 2013*, *Fall 2014, Fall 2015.*

Chemical Structure and Bonding, Intensive (Chem111)—Same as above course, but taught in a 5-day/week format to accommodate students without previous preparation in chemistry. *Fall 2012 (co-taught with F. Blase)*

Chemical Dynamics (Chem112)— A statistical-mechanics based introduction to chemical thermodynamics, equilibrium, electrochemistry and kinetics. Microscopic properties are used to develop basic chemical concepts of energy, enthalpy, entropy, and the Gibbs Energy, and their applications to thermochemistry, equilibria, and electrochemistry. Chemical kinetics, reaction mechanisms, and applications to chemical problems are also discussed. (Freshman level course). *Spring 2017*

Statistical Thermodynamics & Kinetics (Physical Chemistry I) (Chem304)—A quantitative approach to the description and prediction of behavior in chemical systems, with an emphasis on computational approaches. Topics to be covered include: introductory quantum mechanics and energy in molecules, statistical mechanics and energy partitioning, thermodynamics of molecules and larger systems, physical and chemical equilibrium, and chemical kinetics. *Fall 2008, Fall 2009, Fall 2010, Fall 2013, Fall 2016*

Quantum Chemistry (Physical Chemistry II) (Chem305)— The quantum theory of atoms and molecules as applied to problems in molecular structure, computational chemistry, and basic spectroscopic techniques. Emphasis on computational methodology. *Spring 2009, Spring 2010, Spring 2011, Spring 2013, Spring 2014, Spring 2015.*

Laboratory in Chemical Structure and Reactivity ("Junior Superlab") (Chem301)— Two lectures and two laboratory periods per week. An introduction to the methods of research in chemistry. Inorganic, organic, physical chemistry, computational chemistry, and biochemical concepts are integrated in a broad laboratory study of structure and its relationship to chemical reactivity. Physical methods are used in studies of organic, inorganic, and biochemical reactions. Chemical synthesis and the modern methods of computation and instrumental analytical chemistry are particularly stressed. *Fall 2009 (co-taught with R. Scarrow), Fall 2010 (co-taught with K. Åkerfeldt).*

Topics in Materials Science: Semiconductor (Chem353, Chem354) Nanowires—Survey of one-dimensional inorganic semiconducting solids, i.e., "nanowires", structured around synthesis, post-synthetic modifications/doping, and applications, based primarily on readings taken from the literature. Emphasis on physical chemistry principles underlying these phenomena. Spring 2011, Fall 2012, Spring 2015.

Topics in Materials Science: Graphene (Chem353)—Survey of the electronic, optical, and mechanical properties of graphene, with an emphasis on the quantum mechanical origins and computational aspects concerning these properties, based primarily on readings taken from the literature. After the initial class sessions focusing on the quantum mechanics of zero-, one- and two- dimensional solids, survey of: edge states, topological defects, substitutional doping, non-covalent doping, bilayer/trilayer graphene properties, graphane/graphone/fluorographene, and alternative two-dimensional carbon allotropes. *Fall 2012*

Topics in Materials Science: Data-Driven Materials Discovery (Chem353)—Survey of data-driven collaborative approaches for materials discovery and development, motivated in part by the United States' Materials Genome Initiative and similar initiatives world-wide. Review of chemistry and computational methodologies existing projects pertaining to organic, inorganic and nanostructured materials for applications such as gas storage and separation, thermoelectrics, photovoltaics, and electronics based on readings from the literature. Readings and discussion on data-intensive science, "open science", culminating in student proposals for new data-driven/collaborative/online project to assist in chemical/materials discovery. *Spring 2014, Fall 2017*

Publications:

Haverford College (* denotes Haverford undergraduate students)

Books:

J. Schrier, *Introduction to Computational Physical Chemistry* (Mill Valley, California: University Science Books, 2017) 505pp.

Refereed Journal Articles:

P. Racuglia*, K. C. Elbert*, P. D. F. Adler, C. Falk*, M. B. Wenny*, A. Mollo*, M. Zeller, S. A. Friedler, J. Schrier, A. J. Norquist, "Machine learning assisted materials discovery using failed experiments" *Nature* **533,** 73-76 (2016) doi:10.1038/nature17439
[Cover article; coverage in C&E News,Nature News, Scientific American, Wall Street Journal, Engadget, phys.org]

P. D. F. Adler, R. Xu*, J. H. Olshansky*, M. D. Smith*, K. C. Elbert*, Y. Yang*, G. M. Ferrence, M. Zeller, J. Schrier, A. J. Norquist, "Probing structural adaptability in templated vanadium selenites" *Polyhedron* **114**, 184-193 (2016) doi:10.1016/j.poly.2015.11.038

A. Nourmahnad*, M. B. Wenny*, M. Zeller, J. Schrier, A. J. Norquist, "The role of inorganic acidity on templated vanadate composition and dimensionality" *J. Solid State Chem* **236**, 215-221 (2016) doi:10.1016/j.jssc.2015.08.007

S. D. Pineda Flores*, G. C. Martin-Noble*, R. L. Phillips*, J. Schrier, "Bio-inspired Electroactive Organic Molecules for Aqueous Redox Flow Batteries: 1. Thiophenoquinones", *J. Phys. Chem. C*. **119**, 21800-21809 (2015) doi: 10.1021/acs.jpcc.5b05346

G. C. Martin-Noble*, D. Reilley*, Luis M. Rivas*, M.D. Smith*, J. Schrier, "EQeq+C: An Empirical Bond-Order Corrected Extended Charge Equilibration Method", *J. Chem. Theory. Comput.* **11,** 3364-3374 (2015).

A. Nourmahnad*, M. D. Smith*, M. Zeller, G. Ferrence, J. Schrier, A. J. Norquist, "The role of non-covalent interactions on vanadium tellurite chain connectivities", *Inorg. Chem.* **54**, 694-703 (2015)

J. Olshansky*, K. Wiener*, M. D. Smith*, A. Nourmahnad*, M. Charles*, M. Zeller, J. Schrier, A. J. Norquist, "Formation principles for vanadium selenites: the role of pH on product composition" *Inorg. Chem.* **53**, 12027-12035 (2014)

S. Mandrá, J. Schrier, M. Ceotto, "Helium Isotope Enrichment by Resonant Tunneling Through Nanoporous Graphene Bilayers", *J. Phys. Chem. A* **118**, 6457-6465 (2014)

J. H. Koffer*, J. H. Olshansky*, M. D. Smith*, K. J. Hernandez, M. Zeller, G. M. Ferrence, J. Schrier, A. J. Norquist, "Formation principles for templated vanadium selenite oxalates" *Cryst. Growth Des.* **13**, 4504-4511 (2013)

K. Solvik*, J. A. Weaver*, A. M. Brockway*, J. Schrier, "Entropy-driven Molecular Separations in 2D-Nanoporous Materials, with Application to High-performance Paraffin/Olefin Membrane Separations" *J. Phys. Chem. C* **117**, 17050-17057 (2013)

K. B. Chang*, M. D. Smith*, S.M. Blau*, E. C. Glor*, M. Zeller, J. Schrier, A. J. Norquist, "Steric-Induced Layer Flection in Templated Vanadium Tellurites" *Cryst. Growth Des.* **13**, 2190-2197 (2013)

A. M. Brockway*, J. Schrier, "Isotopic and Chemical Separation of Noble Gases using PG-ESX (X=1,2,3) Nanoporous Two-dimensional Polymers" *J. Phys. Chem. C.* **117**, 393-402 (2013).

J. H. Olshansky*, T. T. Tran, K. J. Hernandez, M. Zeller, P. S. Halasyamani, J. Schrier, A. J. Norquist, "Role of Hydrogen-Bonding in the Formation of Polar Achiral and Nonpolar Chiral Vanadium Selenite Frameworks" *Inorg. Chem.* **51**, 11040-11048 (2012).

J. Schrier, "Carbon Dioxide Separation with a Two-Dimensional Polymer Membrane" *ACS Appl. Mater. Interfaces* **4**, 3745-3752 (2012).

A. W. Hauser, J. Schrier, P. Schwerdtfeger, "Helium Tunneling through Nitrogen-Functionalized Graphene Pores: Pressure- and Temperature-Driven Approaches to Isotope Separation" *J. Phys. Chem. C* **116**, 10819-10827 (2012).

M. D. Smith*, S. M. Blau*, K. B. Chang*, T. T. Tran, M. Zeller, P. S. Halasyamani, J. Schrier, A. J. Norquist, "Inducing polarity in $[VO3]^{n}_{n-}$ chain compounds using asymmetric hydrogen-bonding networks" *J. Solid State Chem.* **195**, 86-93 (2012).

J. Schrier, "Ethanol concentration by forward osmosis with solar-regenerated draw solution", *Solar Energy* **86**, 1351-1358 (2012).

J. Schrier, J. McClain*, "Thermally-driven isotope separation across nanoporous graphene" *Chem. Phys. Lett.* **521**, 118-124 (2012).

J. Schrier, "Fluorinated and Nanoporous Graphene Materials As Sorbents for Gas Separations" *ACS Appl. Mater. Interfaces*, **3**, 4451-4458 (2011).

M. D. Smith*, S. M. Blau*, K. B. Chang*, Matthias Zeller, J. Schrier, A. J. Norquist, "Beyond Charge Density Matching: The Role of C–H···O Interactions in the Formation of Templated Vanadium Tellurites" *Cryst. Growth Des.* **11**, 4213-4219 (2011).

A. N. Sokolov, S. Atahan-Evrenk, R. Mondal, H. B. Akkerman, R. S. Sánchez-Carrera, S. Granados-Focil, J. Schrier, S. C.B. Mannsfeld, A. P. Zoombelt, Z. Bao, A. Aspuru-Guzik, "From computational discovery to experimental characterization of a high hole mobility organic crystal" *Nature Commun*. **2**, 437 (2011). doi:10.1038/ncomms1451

J. H. Olshansky*, S. M. Blau*, M. Zeller, J. Schrier, A. J. Norquist, "Understanding an order-disorder phase transition in ionothermally synthesized gallium phosphates" *Cryst. Growth Des.* **11**, 3065-3071 (2011).

E. C. Glor*, S. M. Blau*, J. Yeon, M. Zeller, P. S. Halasyamani, J. Schrier, A. J. Norquist, "[R-$C_7H_{16}N_2$][$V_2Te_2O_{10}$] and [S-$C_7H_{16}N_2$][$V_2Te_2O_{10}$]; new polar templated vanadium tellurite enantiomers" *J. Solid State Chem.* **184**, 1445-1450 (2011)

A. V. Subhas*, J. Whealdon*, J. Schrier, "Predicting organic thin-film transistor carrier type from single molecule calculations" *Comput. Theoret. Chem.* **966**, 70-74 (2011).

J. McClain*, J. Schrier, "Multiple Exciton Generation in Graphene Nanostructures" *J. Phys. Chem. C* **114**, 14332-14338 (2010)

J. Schrier, "Helium Separation Using Porous Graphene Membranes" *J. Phys. Chem. Lett.* **1**, 2284-2287 (2010)

K. B. Chang*, D. J. Hubbard*, M. Zeller, J. Schrier, A. J. Norquist, "The role of stereoactive lone pairs in templated vanadium tellurite charge density matching" *Inorg. Chem.* **49**, 5167-5172 (2010)

R. Sanchez-Carrera, S. Atahan-Evrenk, J. Schrier, A. Aspuru-Guzik, "Theoretical Characterization of the Air-stable, High-mobility Dinaphtho[2,3-b:2',3'-f]thieno[3,2-b]-thiophene Organic Semiconductor" *J. Phys. Chem. C*. **114**, 2334 (2010)

H. S. Casalongue*, S. J. Choyke*, A. N. Sarjeant, J. Schrier, A. J. Norquist, "Charge density matching in templated molybdates" *J. Solid State Chem.* **182**, 1297 (2009)

Lawrence Berkeley National Laboratory

J. Sun, W. E. Buhro, L.-W. Wang and J. Schrier, "Electronic structure and spectroscopy of cadmium telluride quantum wires" *Nano Lett*. **8,** 2913 (2008)

J. Schrier and L.-W. Wang, "Shape dependence of resonant energy transfer between semiconductor nanocrystals", *J. Phys. Chem. C* **112**, 11158 (2008)

J. Schrier, B. Lee and L.-W. Wang, "Mechanical and electronic-structure properties of compressed CdSe tetrapod nanocrystals", *J. Nanosci. Nanotechnol*. **8**, 1994 (2008)

A. Aspuru-Guzik, J. Schrier, S. Granados, "Air-Stable, High Hole Mobility [:4,5]thieno[2,3-d]thiophene Derivatives", US Provisional Patent 60/800,324 (2007).; US Patent PCT/US2008/069970; World Patent WO/2009/009790

L. Fang, J. Y. Park, Y. Cui, A. P. Alivisatos, J. Schrier, B. Lee, L.-W. Wang and M. Salmeron, "Mechanical and electrical properties of CdTe tetrapods studied by atomic force microscopy" *J. Chem. Phys*. **127**, 184704 (2007)

J. Schrier, D. O. Demchenko, L.-W. Wang and A. P. Alivisatos, "Optical properties of ZnO/ZnS and ZnO/ZnTe heterostructures for photovoltaic applications", *Nano Lett*. **7,** 2377-2382 (2007).

J. Schrier and L.-W. Wang, "A systematic first principles study of nanocrystal quantum-dot quantum wells," *Phys. Rev. B* **73**, 245332 (2006).

J. Schrier and L.-W. Wang, "On the Size-Dependent Behavior of Nanocrystal-Ligand Bonds," *J. Phys.* Chem. B **110**, 11982-11985 (2006).

University of California, Berkeley

J. Schrier and K. B. Whaley, "Hyperfine coupling constants of Azafullerenes $C_{19}N$, $C_{59}N$, $C_{69}N$ and $C_{75}N$," *J. Phys. Chem. A* **110**, 5386-5390 (2006).

J. Schrier and K. B. Whaley, "Atomistic theory of coherent spin transfer between molecularly bridged quantum dots," *Phys. Rev. B* **72**, 085320 (2005).

L. Senapati, J. Schrier, and K. B. Whaley, "Electronic transport, structure, and energetics of endohedral $Gd@C_{82}$ metallofullerene", *Nano Lett.* **4**, 2073-2078 (2004).; *ibid*. **5,** 2341 (2005).

J. Schrier and K. B. Whaley, "A simple model for magnetization ratios in doped nanocrystals," *J. Appl. Phys*. **95**, 1436-1438 (2004).

P. J. Bratt, P. Heathcote, A. Hassan, J. van Tol, L. C. Brunel, J. Schrier, and A. Angerhofer, "EPR at 24 T of the primary donor radical cation from Blastochloris viridis", *Chem. Phys.* **294**, 277-284 (2003)

J. Schrier and K. B. Whaley, "Tight-binding g-factor calculations of CdSe nanostructures," *Phys. Rev. B* **67**, 235301 (2003).

St. Peter's College:

P. J. Bratt, O. Poluektov, M. Thurnauer, J. Krystek, L.-C. Brunel, J. Schrier, Y.-W Hsiao, M. Zerner, A. Angerhofer, "The g-factor anisotropy of Plant Chlorophyll a^{*+}", *J. Phys. Chem. B*, **104**, 6973-6977 (2000).

Presentations:

Seminars and Colloquia:

"Discovering the rules of organohalide hybrid perovskite synthesis with machine-learning and high-throughput robotic synthesis", Visiting Faculty Seminar, Lawrence Berkeley National Laboratory, Berkeley, California 02 Aug 2017

"The Dark Reactions Project: Machine Learning-Assisted Materials Discovery to Materials Discovery", Inorganic Nanostructures Group, Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, California, 06 July 2017

"The Dark Reactions Project: Machine Learning-Assisted Materials Discovery using Failed Experiments", Chemistry Seminar, Haverford College, Pennsylvania, 21 April 2017

"The Dark Reactions Project: Machine Learning-Assisted Materials Discovery using Failed Experiments", Philadelphia Theoretical Chemistry Club, Swarthmore College, Pennsylvania, 01 February 2017

"The Dark Reactions Project: Machine Learning-Assisted Materials Discovery using Failed Experiments", Inorganic Nanostructures Group, Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, California, 09 January 2017

"Hunting for Better Aqueous Organic Redox Flow Battery Materials", Harvard University, Cambridge, Massachusetts 05 May 2016

"The Dark Reactions Project: Machine Learning-Assisted Materials Discovery using Failed Experiments", Chemistry Seminar, University of the Pacific, Stockton, California, 05 April 2016

"Gas Separation with '2D' Membranes", Chemical Physics seminar, Fritz Haber Institute, Berlin, Germany, 07 Dec 2015

"The Dark Reactions Project: Learning from 'Failed' Reactions to Accelerate Materials Discovery", Fritz Haber Institute Chemical Physics Departmental Workshop, Schloß Ringberg, 20-25 September 2015

"Dark reaction project: Archiving and deriving value from unreported 'failed' hydrothermal synthesis reactions", Joint Center for Artificial Photosynthesis (JCAP), Lawrence Berkeley National Laboratory (with telecast to Cal-Tech facility), Berkeley, California, 20 August 2014

"Isotopic and chemical separations using nanoporous two-dimensional membranes", Chemistry Seminar, University of Richmond, Virginia, 05 April 2013

"Isotopic and chemical separations using nanoporous two-dimensional membranes", Chemistry Seminar, Wesleyan University, Connecticut, 01 March 2013

"Isotopic and chemical separations using nanoporous two-dimensional membranes", Chemistry Seminar, San Francisco State University, California, 15 Feb 2013

"Quantum Chemical Engineering: The feasibility of isotope separation using quantum tunneling effects", ITAMP/Chemistry Seminar Series, Harvard University, 21 September 2012

"Isotopic and chemical separations using nanoporous two-dimensional membranes", Chemistry Seminar, Clark University, Massachusetts, 20 September 2012

"Isotopic and chemical separations using nanoporous two-dimensional membranes", Quantum Simulations Group, Lawrence Livermore National Laboratory, 06 August 2012

"Isotopic and chemical separations using nanoporous two-dimensional membranes", Molecular Foundry, Lawrence Berkeley National Laboratory, 01 August 2012

"Quantum Chemical Engineering: The feasibility of isotope separation using quantum tunneling effects," Quantum Information Seminar, University of California, Berkeley, 21 March 2012

"Improving Graphene with Scissors and a Hole-Punch", Chemistry Colloquium, Bryn Mawr College, Pennsylvania, 12 November 2010

"'Sculpting' nanomaterial electronic states", Department of Mathematical Physics, National University of Ireland, Maynooth, Ireland, 25 June 2010

"'Sculpting' nanomaterial electronic states", Atlantic Center for Atomistic Modeling, University College, Dublin, Ireland 18 June 2010

"Sculpting quantum states out of graphene nanoribbons", Haverford College, 23 June 2009

"Understanding nanostructures from the atoms up", St. Peter's College, New Jersey, 12 Feburary 2009

"Designing photovoltaic nanostructures using atomistic simulations", Chemistry Department, Brown University, 21 Jan 2008

"Designing photovoltaic nanostructures using atomistic simulations", Chemistry Department Haverford College, 19 Nov 2007

"Using High Performance Computing to Design Solar Energy Materials", Scientific Computing Seminar, Lawrence Berkeley National Laboratory, 19 Oct 2007

"Spins in Tight Places: Theoretical studies of spin properties in nanocrystals and fullerenes", Scientific Computing Seminar, Lawrence Berkeley National Laboratory, 7 Mar 2005

National Meetings and Conferences:

"Dark Reactions Project: Undergraduate-driven discovery of new materials with cheminformatics, machine learning, and experiments (and robots) at a small liberal arts college", 254th American Chemical Society National Meeting, Washington, D.C., 24 Aug 2017

"Introduction to Computational Physical Chemistry: Integrating computational method development into the standard undergraduate physical chemistry curriculum," 254th American Chemical Society National Meeting, Washington, D.C., 21 Aug 2017

"Dark reactions project: A machine learning approach to materials discovery", 253nd American Chemical Society National Meeting, San Francisco, 02 Apr 2017

"Dark Reactions Project: Machine learning-assisted materials discovery using failed experiments" 252nd American Chemical Society National Meeting, Philadelphia, 25 Aug 2016

"Using drug discovery methods to accelerate the search for better battery materials" 251st American Chemical Society National Meeting, San Diego, 14 Mar 2016

"Bioinspired electroactive organic molecules for aqueous redox flow batteries" International Chemical Congress of Pacific Basin Societies ("Pacifichem"), Honolulu, 18 December 2015

"Bilayer silicatene: Glassy defect structures and gas separation properties" International Chemical Congress of Pacific Basin Societies ("Pacifichem"), Honolulu, 17 December 2015

"Helium isotope enrichment by resonant tunneling through nanoporous graphene bilayers", 248th American Chemical Society National Meeting, San Francisco, 13 August 2014

"EQeq+C: An empirical bond-order corrected extended charge equilibration method", 248th American Chemical Society National Meeting, San Francisco, 13 August 2014

"Using surface adsorption and entropic barriers to improve gas separation by 2D nanoporous membranes", 247th American Chemical Society National Meeting, Dallas, 18 March 2014

"Dark reaction project: Archiving and deriving value from unreported "failed" hydrothermal synthesis reactions", 247th American Chemical Society National Meeting, Dallas, 17 March 2014

"How fast is gas separation through a nanoporous graphene membrane? The role of surface adsorption, and application to post-combustion CO_2 capture", 244th American Chemical Society National Meeting, Philadelphia, 21 August 2012

"Isotope separation using quantum tunneling", 244th American Chemical Society National Meeting, Philadelphia, 21 August 2012

"Thermally-driven Isotope Separation Across Nanoporous Graphene", American Physical Society March Meeting, Boston, 29 February 2012

"Forster resonant energy transfer between CdSe nanocrystals: An empirical pseudopotential/transition density cube approach", American Physical Society March Meeting, New Orleans, 11 Mar 2008.

"Mechanical and electronic properties of semiconductor nanocrystalline tetrapods", American Chemical Society 234th National Meeting, Boston, 21 Aug 2007.

"Air-stable, high performance, rigid [:4,5]thieno[2,3-d]thiophene- derivative organic semiconductors", American Chemical Society 234th National Meeting, Boston, 19 August 2007.

"Optical properties of ZnO/ZnS and ZnO/ZnTe heterostructures for photovoltaic applications", American Physical Society March Meeting, Denver, 05 Mar 2007.

"Applications of the charge patching approach to individually heterostructured semiconductor nanocrystals", American Chemical Society 232nd National Meeting, San Francisco, 11 Sept 2006. (Winner: "Emerging Technologies in Computational Chemistry" award)

"A charge patching method calculation of a quantum dot/quantum well nanosystem", American Physical Society March Meeting, Baltimore, 13 Mar 2006.

"The charge patching density functional approach for semiconductor nanostructures", Bay Area Scientific Computing Day, Lawrence Livermore National Laboratory, 4 Mar 2006.

"Microscopic Analysis of Spin Coherences in Semiconductor Nanostructures", Army Research Office Quantum Computing Program Review, 18-22 Aug 2003.

Outreach Talks:

"Das ‚Dark Reactions' Projekt" (in German), Goethe-Institut, Bonn, Germany, 18 July 2016

"Careers in Science", Academy One Public School (6th-8th grade), Jersey City, NJ, 20 June 2014

Research Students Supervised at Haverford College (by starting academic year/summer):

2017: Liana Alves '18, Xiwen Jia '19, Aaron Schankler '18, Gregry Van Aken '19, Qingyang Zhang '18

2016: Xiwen Jia '19, Tristan Pepin '18, Malia Wenny '17

2015: Raghav Bali '18, Daniel Hopkins '16, Geoffrey Martin-Noble '16, Richard Phillips '18, David Reilley '16, Bradley Studnitzer '17, Julian Taylor '18, Malia Wenny '17, Jiaming Xu '18, Bowen Yao '17

2014: Jade Andrade '15, John Curry '15, Geoffrey Martin-Noble '16, Aurelio Mollo '17, Sergio Pineda Flores '15, David Reilley '16, Kylen Solvik '15, Malia Wenny '17, Bowen Yao '17

2013: Jade Andrade '15, Avi Bregman '14, Casey Falk '16, Geoffrey Martin-Noble '16, Anahita Nourmahnad '14, David Reilley '16, Luis Rivas '16, Kylen Solvik '15

2012: Jade Andrade '15, Grace Cheong '13, Matthew Holmes '15, Anahita Nourmahnad '14, Matthew Smith '13, Kylen Solvik '15, Jessica Weaver '13, Jennifer Whealdon '13

2011: Samuel Blau '12, Anna Brockway '12, Malenca Logan '14, Matthew Smith '13, Arman Terzian '14, Jennifer Whealdon '13

2010: Samuel Blau '12, Anna Brockway '12, Ethan Glor '11, James McClain '11, Matthew Stern '11, Jennifer Whealdon '13

2009: Connor Bischak '10, Kelvin Chang '10, Anna Brockway '12, James McClain '11, Alexander Vargo '12

2008: Ethan Alguire '09, Gregory Guthe '09, Adam Subhas '09

Senior Theses Advised at Haverford College (by graduation year, alphabetical by surname):

Malia Wenny ’17, “Probing the synthesis-structure relationship in organohalide perovskites” (joint with Alexander Norquist)

Geoffrey Martin-Noble ’16, “Optimizing a Machine Learning System for Materials Discovery” (joint with Sorelle Friedler)

David Reilley ’16, “A Computational Study of the Stereospecificity of the Lubell Method for the Synthesis of Azabicycloalkanone Amino Acids”

Jade T. Andrade ’15, “Computational Studies of Zinc Finger Proteins: Molecular Dynamics Simulations and Deriving Force Field Parameters for Other M(II) Metals”

John O. Curry ’15, “An Investigation into the Quantum-Mechanical Gas Separation Properties of Silicatene”

Kylen Solvik ’15, “Noble gas adsorption to the 2DCN, 2DSP, CTF-0, and PG two-dimensional gas separating membranes”

Sergio Pineda Flores ’15, “Quantum Chemical Screening of Bio-Inspired Redox Species for Organic Redox Flow Battery Design”

Avi Bregman ’14, “Charge Transport Properties of Doped Nano Graphene Bowties”

Anahita Nourmahnad ’14, “An Investigation of Structure-directing Influences in Organically Templated Vanadium Oxo Chain Connectivities” (joint with Alexander Norquist)

Grace Cheong ’13, “Computational Studies of Potential Energy Surfaces of Graphene and Nanoporous Graphene Analogues as Separation Membranes”

Matthew Smith ’13, “Understanding the Structure, Charge, and Properties of Templated Vanadium Oxysalts” (joint with Alexander Norquist)

Jessica Weaver ’13, “The Impactor Factor: The Feasibility of Nanoporous Graphene Design Using Molecular Drills”

Jennifer Whealdon ’13, “Reorganization Energy Minimization in Graphene Nanoparticles: Discovering Novel Candidates for Organic Semiconductor Applications”

Anna Brockway ‘12, “Computational Studies of Quantum Gas Transmission Through Nanoporous Graphene Membranes”

Samuel Blau ‘12, “Lattice Density-Functional Theory for the Hubbard Model of Graphene Nanostructures”

James McClain ‘11, “Multiple Exciton Generation in Graphene Nanoparticles and Thermally-driven Isotope Separation by Quantum Tunneling”

Matthew Stern ‘11, “Quantum chemical analysis of β-thiocyanatoalanine: a novel (residue) approach to determining local protein dynamics”

Connor Bischak ‘10 "Comparison of computational and experimental study of isothiocyanate infrared probes" (joint with Casey Londergan)

Ethan Alguire ‘09, "An investigation of the Ragot-Cortona correlation functional"

Gregory Guthe ‘09 "Modeling $TPPS_4$ Aggregation with Molecular Dynamics" (joint with Walter Smith)

Adam Subhas ‘09, "Modeling the Self-Assembly and Optical Properties of Meso-Tetrakis(4-Sulfonatophenyl)Porphine using Density Functional Theory"