

Joshua A. Schrier
Assistant Professor of Chemistry

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Education **University of California, Berkeley** Berkeley, CA
Ph.D. in Chemistry 5/2005
St. Peter's College Jersey City, NJ
BS *Summa Cum Laude* in Chemistry 5/2000

Training **Lawrence Berkeley National Laboratory** Berkeley CA
Postdoctoral fellow for Lin-Wang Wang 5/2005-7/2008
University of California, Berkeley Berkeley, CA
Graduate student of K. Birgitta Whaley 9/2000-5/2005

Grants and Awards

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 2009-2011
Undergraduate New Investigator Award

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

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

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

University of California, Berkeley 2001
Abramson Graduate Scholarship

Barry M. Goldwater Scholar 1999

Service

-Haverford College

Research advisor for 6 graduated and 4 current students (2008-present)
Environmental Studies Concentration working group (2009-2010)
Committee for Environmental Responsibility (2009-present)
Scientific Computing Concentration Coordinator (2010-2011)
Scientific Computing Concentration Chemistry Representative (2009-present)
Bryn Mawr Geochemistry Search Committee (2010-2011)
Laboratory and Biosafety Committee (2010-2011)

-Scientific Community (past 3 years)

Ad hoc reviewer for: *ACS Nano*; *Am. J. Phys.*; *Chemistry of Materials*; *Journal of Chemical Physics*; *Journal of Physical Chemistry A / B/C/Lett.*; *Journal of Physics D: Applied Physics*; *Journal of Nanoscience and Nanotechnology*; *Physical Review A / B*

Proposal reviewer for: U. S. Dept of Energy—Physical Behavior of Materials(BES) (2011); National Science Foundation (2010); Center for Materials Innovation, Washington University—St. Louis (2010); Irish Centre for High-End Computing Class A allocation awards (2009); U.S. Dept. of Energy--Basic Energy Sciences (2008); U.S. Dept. of Energy Innovative and Novel Computational Impact on Theory and Experiment (INCITE) computer allocation (2008)

Publications:

Haverford College (* denotes Haverford undergraduate students)

- 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-C₇H₁₆N₂][V₂Te₂O₁₀] and [S-C₇H₁₆N₂][V₂Te₂O₁₀]; new polar templated vanadium tellurite enantiomers" *J. Solid State Chem.* **184**, 1445 (2011)
- A. V. Subhas*, J. Whealdon*, J. Schrier, "Predicting organic thin-film transistor carrier type from single molecule calculations" *Comput. Theoret. Chem.* **966**, 70 (2011).
- J. McClain*, J. Schrier, "Multiple Exciton Generation in Graphene Nanostructures" *J. Phys. Chem. C* **114**, 14332 (2010)
- J. Schrier, "Helium Separation Using Porous Graphene Membranes" *J. Phys. Chem. Lett.* **1**, 2284 (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 (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).
- 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).

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

(2011)

- James McClain, "Multiple Exciton Generation in Graphene Nanoparticles and Thermally-driven Isotope Separation by Quantum Tunneling"
- Matthew Stern, "Quantum chemical analysis of β -thiocyanatoalanine: a novel (residue) approach to determining local protein dynamics"

(2010)

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

(2009)

- Ethan Alguire, "An investigation of the Ragot-Cortona correlation functional"
- Gregory Guthe (joint with Walter Smith): "Modeling TPPS₄ Aggregation with Molecular Dynamics"
- Adam Subhas, "Modeling the Self-Assembly and Optical Properties of Meso-Tetrakis(4-Sulfonatophenyl)Porphine using Density Functional Theory"