Curriculum Vitae -- July 02008

Joshua A. Schrier
Haverford College
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Education:

Ph.D. in Theoretical Physical Chemistry
University of California, Berkeley (2000-2005)

BS/BS Summa Cum Laude Chemistry and Biochemistry, Music Minor
Saint Peter's College (1996-2000)

Prizes and Awards:

Luis W. Alvarez Postdoctoral Fellowship in Computational Sciences
(2005-2006)

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

National Semiconductors NATCAR Autonomous robotic car racing competition,
First Prize, May 2004

United States Army Research Office Quantum Computing Graduate Research
Fellow (QuaCGR), (2001-2003)

Abramson Graduate Scholarship (2001)

Barry M. Goldwater Scholar (1999)

Research Experience:

(2008-present) Assistant Professor of Chemistry, Haverford College,
Pennsylvania. Research efforts in theoretical methods for atomistic
treatment of semiconductor nanocrystal and nanowire photovoltaics and
thermoelectrics.

(2005-2008) Postdoctoral fellow, Computational Research Division,
Lawrence Berkeley National Laboratory. Development and application
of high performance parallel plane wave pseudopotential density
functional methods for treating multi-thousand atom semiconductor
nanostructures, under the direction of Dr. Lin-Wang Wang.

(2000-2005) Ph.D. Graduate Research, Department of Chemistry, UC
Berkeley. Development of theoretical methods for the
magneto-optical, transport, and magnetic properties semiconductor
nanostructures and endohedral fullerenes, under the direction of
Prof. K. Birgitta Whaley.

(1999) Summer Undergraduate Research, University of Florida--Quantum Theory Project. Application of Electron Spin Resonance (ESR) g-factor calculations to the prediction of chlorophyll a and special-pair bacteriochlorophyll dimer structures, under the direction of Profs. Michael C. Zerner and Alexander Angerhofer.

(1998) Summer Undergraduate Research, University of Connecticut. Development of preparative HPLC protocol for purification of lycopene, under the direction of Prof. Harry A. Frank.

Oral Presentations:

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

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

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

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

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

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

"Optical properties of ZnO/ZnS and ZnO/ZnTe heterostructures for photovoltaic applications", American Physical Society March Meeting, 5 Mar 2007.

"Applications of the charge patching approach to individually heterostructured semiconductor nanocrystals", American Chemical Society 232nd National Meeting, 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, 13 Mar 2006.

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

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

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

Publications:

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

J. Schrier and L.-W. Wang, "Shape dependence of resonant energy transfer between semiconductor nanocrystals", J. Phys. Chem. C (in press) doi: 10.1021/jp800489m

J. Schrier, S. Atahan, and A. Aspuru-Guzik, "Properties of [:4,5]thieno[2,3-d]thiophene derivatives for organic field effect transistor applications" (submitted J. Am. Chem. Soc.)

J. Schrier, B. Lee and L.-W. Wang, "Mechanical and electronic-structure properties of compressed CdSe tetrapod nanocrystals", J. Nanosci. Nanotechnol. 8, 1994 (2008) ; LBNL-62312.

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) ; doi:10.1063/1.2786993 ; LBNL-62361 (VJ Nano)

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). doi:10.1021/nl071027k ; LBNL-62616. (10th-most accessed paper in Nano Lett. in the 3rd quarter of 2007)

J. Schrier and L.-W. Wang, "A systematic first principles study of nanocrystal quantum-dot quantum wells," Phys. Rev. B 73, 245332 (2006). doi:10.1103/PhysRevB.73.245332 ; LBNL-60838 (VJ Nano)

J. Schrier and L.-W. Wang, "On the Size-Dependent Behavior of Nanocrystal-Ligand Bonds," J. Phys. Chem. B 110, 11982-11985 (2006). doi:10.1021/jp061117y ; LBNL-59148

J. Schrier and K. B. Whaley, "Hyperfine coupling constants of Azafullerenes C19N, C59N, C69N and C75N," J. Phys. Chem. A 110, 5386-5390 (2006). doi:10.1021/jp056462m (John. C. Light Festschrift); LBNL-59152

J. Schrier and K. B. Whaley, "Atomistic theory of coherent spin transfer between molecularly bridged quantum dots," Phys. Rev. B 72, 085320 (2005). doi:10.1103/PhysRevB.72.085320 (VJ Nano; VJ Ultrafast)

L. Senapati, J. Schrier, and K. B. Whaley, "Electronic transport, structure, and energetics of endohedral Gd@C82 metallofullerene", Nano Lett. 4, 2073-2078 (2004). doi:10.1021/nl049164u ; ibid. 5, 2341 (2005). doi:10.1021/nl0518831

J. Schrier and K. B. Whaley, "A simple model for magnetization ratios in doped nanocrystals," J. Appl. Phys. 95, 1436-1438 (2004). doi:10.1063/1.1637708

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). doi:10.1016/S0301-0104(03)00281-7

J. Schrier and K. B. Whaley, "Tight-binding g-factor calculations of CdSe nanostructures," Phys. Rev. B 67, 235301 (2003). doi:10.1103/PhysRevB.67.235301 (VJ Nano)

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(30), 6973-6977 (2000). doi:10.1021/jp001126l

Patents:

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).

Professional Society Memberships:

American Chemical Society (ACS)
American Physical Society (APS)
American Association for the Advancement of Science (AAAS)

Professional Service:

Peer review referee for:
- ACS Nano;
- Chemistry of Materials;
- Journal of Chemical Physics;
- Journal of Physical Chemistry A / B;
- Journal of Physics D: Applied Physics;
- Journal of Nanoscience and Nanotechnology;
- Physical Review A / B;
- Supercomputing 2006 (proceedings)

Proposal review for:
- Department of Energy--Basic Energy Sciences (2008)
- Innovative and Novel Computational Impact on Theory and Experiment (INCITE) 2007, 2008
- National Energy Research Scientific Computing (NERSC) Allocations, 2008.

Conference service:
- Presider, "INOR: Nanoscience: Synthesis and Characterization: Rods and Fiber", ACS 234th National Meeting, 2007.
- Chairman, "Focused Session: Computational Nanoscience II", APS March meeting, 2006.

Consortium/Workshop participation:
- Frontiers of Extreme Computing 2007 ("Zettaflops"), Santa Barbara, CA, 21-25 Oct 2007.

Research Interests:

Electronic structure theories of nanostructures; semiempirical and ab initio quantum chemistry; density functional theory; plane-wave methods; colloidal semiconductor nanocrystals (colloidal quantum dots); fullerenes and endohedral fullerenes; electron and nuclear spin resonance spectroscopies; asteroid occultations; solar energy utilization; electronic materials; photovoltaic materials; thermoelectric materials; computational nanoscience

References:

Dr. Lin-Wang Wang (Postdoctoral Advisor)
Lawrence Berkeley National Laboratory
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Berkeley, CA 94720
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Prof. K. Birgitta Whaley (PhD Thesis Advisor)
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Department of Chemistry
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Prof. Robert A. Harris (PhD Thesis Committee Chairman)
117 Lewis Hall
Department of Chemistry
University of California
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Prof. Alan Aspuru-Guzik (Collaborator)
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