

# Guenter Schneider

## Education

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- Ph.D. (1999)** in Physics, Oregon State University, Corvallis, OR. GPA 4.0/4.0  
Thesis: Calculation of Magnetocrystalline Anisotropy  
**Ph.D. Adviser: Henri J. F. Jansen**
- Diploma (1994)** in Electrical Engineering, University of Stuttgart, Germany.  
Thesis: Modeling an Electron Cyclotron Resonance Heated (ECRH) Silane Plasma  
**Diploma Thesis Adviser: K. Behringer**

## Professional Appointments

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- Sep 2008-Present Assistant Professor — Department of Physics, Oregon State University
- Sep 2006-Aug 2008 Fixed Term Assistant Professor — Department of Physics, Oregon State University
- 2004-2006 Postdoctoral researcher — Department of Physics, University of Karlsruhe, Germany. **Postdoctoral Adviser: Peter Wölfle**
- 2002-2003 Postdoctoral researcher — Center for Computational Materials Science, University of Vienna and Vienna University of Technology, Austria.  
**Postdoctoral Advisers: Joseph Redinger and Raimund Podlucky**
- 1999-2002 Postdoctoral researcher — Department of Physics, Brookhaven National Laboratory, Upton, NY.  
**Postdoctoral Advisers: Michael Weinert and Richard E. Watson**
- 1994-1998 Graduate Research Assistant — Department of Physics, Oregon State University
- 1993-1994 Teaching Assistant — Department of Physics, Oregon State University

## Publications

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23. Geneva Laurita-Plankis, Jason Vielma, Florian Winter, Romain Berthelot, Alain Largeteau, Rainer Pöttgen, **G. Schneider**, M. A. Subramanian, From  $\text{Ag}_2\text{Sb}_2\text{O}_6$  to  $\text{Cd}_2\text{Sb}_2\text{O}_7$ : Investigations on an anion-deficient to ideal pyrochlore solid solution, *J. Solid State Chem.*, **210**, 65-73 (2014).
22. D.H. Foster, F.L. Barras, J. Vielma, and **G. Schneider**, Defect physics and electronic properties of  $\text{Cu}_3\text{PSe}_4$  from first principles, *Phys. Rev. B*, **88**, 195201 (2013).
21. J. M. Vielma and **G. Schneider**, Shell model of  $\text{BaTiO}_3$  derived from ab-initio total energy calculations, *J. Appl. Phys.*, **114**, 174108 (2013).
20. David H. Foster, Timothy Costa, Malgorzata Peszynska, and **Guenter Schneider**, Multiscale modeling of solar cells with interface phenomena, *J. Coupled Syst. Multiscale Dyn.*, **1**, 179-204 (2013).
19. Sean Muir, Jason Vielma, **Guenter Schneider**, Arthur W. Sleight, and Mas Subramanian, The hunt for  $\text{LaFeSbO}$ : synthesis of  $\text{La}_2\text{SbO}_2$  and a case of mistaken identity, *J. Solid State Chem.*, **185**, 156-159 (2012).
18. D.H. Foster, V. Jieratum, R. Kykyneshi, D.A. Keszler, and **G. Schneider**, Electronic and optical properties of potential solar absorber  $\text{Cu}_3\text{PSe}_4$ , *Appl. Phys. Lett.*, **99**, 181903 (2011).
17. A. Zakutayev, J. Tate, and **G. Schneider**, Defect physics of  $\text{BaCuChF}$  ( $\text{Ch}=\text{S, Se, Te}$ ) p-type transparent conductors, *Phys. Rev. B*, **82**, 195204 (2010).
16. A. Branschädel, **G. Schneider**, and P. Schmitteckert\*, Conductance of inhomogeneous systems: Real-time dynamics, *Annalen Der Physik*, **522**, 657-678 (2010).

15. A. Zakutayev, D.H. McIntyre, **G. Schneider**, R. Kykyneshi, D.A. Keszler, C.-H. Park, and J. Tate\*, Tunable properties of wide-band gap p-type BaCu(Ch<sub>1-x</sub>Ch'<sub>x</sub>)F (Ch = S, Se, Te) thin-film solid solutions, *Thin Solid Films*, **518**, 5494-5500 (2010).
14. A. Zakutayev, R. Kykyneshi, **G. Schneider**, D.H. McIntyre, and J. Tate\*, Electronic structure and excitonic absorption in BaCuChF (Ch=S, Se, and Te), *Phys. Rev. B*, **81**, 155103 (2010).
13. Landon Prisbrey, **Guenter Schneider**, and Ethan Minot\*, Modeling the Electrostatic Signature of Single Enzyme Activity, *J. Phys. Chem. B*, **114**, 3330-3333 (2010).
12. A. Bagrets, R. Werner, F. Evers\*, **G. Schneider**, D. Schooss, and P. Wölfle, Lowering of surface melting temperature in atomic clusters with a nearly closed shell structure, *Phys. Rev. B*, **81**, 075435 (2010).
11. M. Weinert\*, **G. Schneider**, R. Podloucky, and J. Redinger, FLAPW: Applications and Implementations, *J. Phys.: Condens. Matter*, **21**, 084201 (2009).
10. J.A. Spies, R. Schafer, J.F. Wager\*, P. Hersh, H. Platt, D.A. Keszler, **G. Schneider**, R. Kykyneshi, J. Tate, X. Liu, A.D. Compaan, and W.N. Schafarman, pin Double-Heterojunction Thin-Film Solar Cell p-layer Assessment, *Solar Energy Materials & Solar Cells*, **93**, 1296 (2009).
9. R. Werner\*, M. Wanner, **G. Schneider**, D. Gerthsen, Island formation and dynamics of gold clusters on amorphous carbon films, *Phys. Rev. B*, **72**, 045426 (2005).
8. C. Deisl, K. Swamy, N. Memmel, E. Bertel, C. Franchini, **G. Schneider**, J. Redinger, S. Walter, L. Hammer, and K. Heinz\*, (3×1)-Br/Pt(110) structure and the charge-density-wave-assisted c(2×1) to (3×1) phase transition, *Phys. Rev. B*, **69**, 195405 (2004).
7. H. Michor, M. El-Hagary, M. Della Mea, M. Piepper, M. Reissner, G. Hilscher, S. Khmelevskyi, P. Mohn, **G. Schneider**, G. Giester and P. Rogl\*, Itinerant electron metamagnetism in LaCo<sub>9</sub>Si<sub>4</sub>, *Phys. Rev. B*, **69**, 081404(R) (2004).
6. R. F. Klie, Y. Zhu\*, **G. Schneider**, and J. Tafto, Experimental probing of the anisotropy of the empty p states near the Fermi level in MgB<sub>2</sub>, *Appl. Phys. Lett.*, **82**, 4316 (2003).
5. Y. Zhu\*, A.R. Moodenbaugh, **G. Schneider**, J.W. Davenport, T. Vogt, Q. Li, G. Gu, D.A. Fischer, and J. Tafto, Unraveling the symmetry of the hole states near the Fermi level in the MgB<sub>2</sub> superconductor, *Phys. Rev. Lett.*, **88**, 247002 (2002).
4. C. McGuinness, K.E. Smith, S.M. Butorin, J.H. Guo, J. Nordgren, T. Vogt, **G. Schneider**, J. Reilly, J.J. Tu, P.D. Johnson\*, and D.K. Shuh, High resolution x-ray emission and absorption study of the valence band electronic structure of MgB<sub>2</sub>, *Europhysics Letters*, **56**, 112 (2001).
3. T. Vogt\*, **G. Schneider**, J.A. Hriljac, G. Yang, and J.S. Abell, Compressibility and electronic structure of MgB<sub>2</sub> up to 8 GPa, *Phys. Rev. B*, **63**, 220505(R) (2001).
2. **G. Schneider** and H.J.F. Jansen\*, Role of orbital polarization in calculations of the magnetic anisotropy, *J. Appl. Phys.*, **87**, 5875 (2000).
1. **G. Schneider**, R.P. Erickson, and H.J.F. Jansen\*, Calculation of the magnetocrystalline anisotropy energy using a torque method, *J. Appl. Phys.*, **81**, 3869 (1997).

## Invited book chapters

2. Peter Schmitteckert and **Guenter Schneider**, Signal Transport and Finite Bias Conductance in and Through Correlated Nanostructures in *High Performance Computing in Science and Engineering '06*, Edited by W.E. Nagel, W. Jäger, and M. Resch, Springer (2007).
1. H.J.F. Jansen, **G. Schneider**, and H.Y. Wang, Calculation of magnetocrystalline anisotropy in transition metals in *Electronic Structure and Magnetism of Complex Materials*, Edited by D. Singh, Springer (2003).

## Presentations

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1. (scheduled) APS March Meeting Denver, CO. *Structure band-gap correlations in semiconductors: Implications for computational band gap prediction.*(March 2014)
2. (scheduled) APS March Meeting Denver, CO. *Band alignment and interface charge decomposition for abrupt and polar-compensated Si/ZnS interfaces.* (March 2014)
3. (scheduled) APS March Meeting Denver, CO. *Optical, electronic and transport properties of tetrahedrites.* (March 2014)
4. SIAM Annual Meeting, San Diego, CA. *Domain Decomposition for Interface Equations with Nonhomogeneous Jumps for Modeling Solar Cells* (poster). (July 2013)
5. APS March Meeting Baltimore, MD. *Calculated Stability and Band Offsets for Compensated and Abrupt Polar Si/Zn(S,Se) (111) Interfaces.* (March 2013)
6. APS March Meeting Baltimore, MD. *Ab-Initio Study of Defect Physics for Layered LaCuChO and BaCuChF (Ch={S,Se,Te}) Structures.* (March 2013)
7. APS March Meeting Baltimore, MD. *Ab-Initio Study of Excitonic Absorption for Layered LaCuChO and BaCuChF (Ch={S,Se,Te}) Structures.* (March 2013)
8. Material Science Institute Fall Conference, University of Oregon, Eugene, OR. *Electron killing defects in solar-region absorber Cu<sub>3</sub>PSe<sub>4</sub>.* (September 2012)
9. Gordon Research Conference on Defects in Semiconductors, Biddeford, ME. *Electron killing defects in solar-region absorber Cu<sub>3</sub>PSe<sub>4</sub>.* (August 2012)
10. Gordon Conference on Solid State Chemistry, New London, NH: *From AgSbO<sub>3</sub> to Cd<sub>2</sub>Sb<sub>2</sub>O<sub>7</sub>: Investigations on a defect to ideal pyrochlore solid solution* (poster). (July 2012)
11. APS March Meeting, Boston, MA. *Structure, stability, and defect analysis of potential solar absorber Cu<sub>3</sub>PSe<sub>4</sub>.* (February 2012)
12. APS March Meeting, Boston, MA. *Growth conditions of oxypnictide compounds LaFePnO Pn={P,As,Sb}.* (February 2012)
13. APS March Meeting, Boston, MA. *First principles study of optical and electronic properties of anthradithiophene based organic conductors.* (February 2012)
14. APS March Meeting, Boston, MA. *Application of Gaussian Approximation Potentials to Barium Titanate* (poster). (February 2012)
15. 13<sup>th</sup> Annual Meeting of the Northwest Section of the APS Meeting, Corvallis, OR. *Optical and electronic properties of potential solar absorber Cu<sub>3</sub>PSe<sub>4</sub>.* (October 2011)

16. 13<sup>th</sup> Annual Meeting of the Northwest Section of the APS Meeting, Corvallis, OR. *First principles study of optical and electronic properties of anthradithiophene based organic conductors*. (October 2011)
17. 13<sup>th</sup> Annual Meeting of the Northwest Section of the APS Meeting, Corvallis, OR. *Shell Model of BaTiO<sub>3</sub> derived from ab-initio DFT Calculations*. (October 2011)
18. **(Invited)** ICIAM 2011 (International Council for Industrial and Applied Mathematics), Vancouver, BC. *Modeling HALL solar cells. HALL = Heterojunction assisted impact ionization*. (July 2011)
19. The 66<sup>th</sup> Northwest Regional Meeting of the American Chemical Society, Portland, OR. *Synthesis and Electrooptical Characterization of Cu<sub>3</sub>PQ<sub>4</sub> (Q = S, Se)* (poster). (June 2011)
20. MRS Spring Meeting, San Francisco, CA. *Native point defects and grain boundaries in wide-bandgap p-type semiconductor BaCuChF (Ch = S, Se, Te)*. (April 2010)
21. APS March Meeting, Portland, OR. *Origin of p-type conductivity in wide band gap BaCuQF (Q=S,Se,Te) semiconductors*. (March 2010)
22. APS March Meeting, Portland, OR. *First principles study of p-type conductivity in wide band gap Cu<sub>3</sub>TaQ<sub>4</sub> (Q=S,Se,Te) semiconductors*. (March 2010)
23. APS March Meeting, Portland, OR. *Shell model for BaTiO<sub>3</sub>-Bi(Zn<sub>1/2</sub>Ti<sub>1/2</sub>)O<sub>3</sub> perovskite solid solutions*. (March 2010)
24. APS March Meeting, Portland, OR. *Persistent interlayer coupling by an antiferromagnetic spacer above its Neel temperature (a Monte Carlo study)*. (March 2010)
25. APS March Meeting Pittsburgh, PA. *Monte Carlo simulation of incommensurate helical ordering in a frustrated FCC lattice of Heisenberg spins*. (March 2009)
26. APS March Meeting Pittsburgh, PA. *Electrostatic signatures of single protein dynamics for detection with carbon nanotube sensors*. (March 2009)
27. 10<sup>th</sup> Annual Meeting of the Northwest Section of the APS Meeting, Portland, OR. *Island formation and dynamics of gold clusters on amorphous carbon films*. (May 2008)
28. APS March Meeting, New Orleans, LA. *Materials for Transparent Electronics: Ab initio calculation of wide bandgap semiconductor interfaces*. (March 2008)
29. APS March Meeting, New Orleans, LA. *Effect of spin-orbit coupling on excitonic levels in layered chalcogenide-fluorides* presented by a student of my collaborator J. Tate, A. Zakutayev. (March 2008)
30. **(Invited)** APS March Meeting, Denver, CO. *Signal transport and finite bias conductance in and through correlated nanostructures*. (March 2007)
31. **(Invited)** 384. WEH Workshop on 'Nonequilibrium Transport of Strongly Correlated Systems: Towards Simulation of Novel Devices', Bad Honnef, Germany. *Conductance in strongly correlated 1D systems: Real-Time Dynamics in DMRG*. (February 2007)

## Invited colloquia and seminars (since September 2006)

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- Oct 14, 2013 – Oregon State University, Physics Colloquium:  
“Understanding Molecules and Solids Bit by Bit”
- Sep 19, 2013 – Temple University, Philadelphia, Pennsylvania – Physics Colloquium:  
“New Semiconductors for a Clean Energy Future: From Basic Properties to  
Computational Materials Design”
- Sep 13, 2013 – University of Wisconsin-Milwaukee, Milwaukee, Wisconsin – Physics Colloquium:  
“New Semiconductors for a Clean Energy Future: From Basic Properties to  
Computational Materials Design”
- May 29, 2013 – Oregon State University, Physics Seminar:  
“Doping and Defects in Complex Semiconductors”
- Mar 15, 2013 – Willamette University, Salem, Oregon – Physics Seminar:  
“New Materials for a Clean Energy Future: From Basic Properties to  
Computational Materials Design”
- Nov 12, 2012 – Oregon State University, Physics Colloquium:  
“New Materials for a Clean Energy Future: From Basic Properties to  
Computational Materials Design”
- Dec 12, 2011 – University of New South Wales – Canberra, Australia, Physics Seminar:  
“From computing materials properties to designing new materials for a cleaner energy future”
- Oct 30, 2009 – Oregon State University, Applied Mathematics Seminar:  
“Computational Materials Design”
- Apr 18, 2008 – Oregon State University, Physics Colloquium:  
“Material Design Challenges in Photovoltaics”
- Feb 22, 2008 – Oregon State University, Materials Science Seminar:  
“Perspectives in Computational Materials Science”
- Oct 5, 2007 – Oregon State University, Applied Mathematics Seminar:  
“Density Matrix Renormalization Group”
- Jan 7, 2007 – University of Karlsruhe, Karlsruhe, Germany, Theory of Condensed Matter Seminar:  
“The melting transition of small metal clusters”
- Oct 30, 2006 – Oregon State University, Physics Colloquium:  
“Melting Transition of Metal Clusters and Transport in 1D Systems”

## Funding

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1. Enhanced Photovoltaic Efficiency through Heterojunction Assisted Impact Ionization  
PI: Kevan (UO), co-PIs: Cohen, Richmond, Rockett, **Schneider**, Tate, Peszynska  
National Science Foundation 9/1/2010 - 8/31/2014  
\$1,500,000
2. Match to: Enhanced Photovoltaic Efficiency through Heterojunction Assisted Impact Ionization  
PIs: **Schneider**, Tate, Peszynska 2011 - 2014 ONAMI \$67,000
3. Phase 2 Real-Time Monitoring of Trace Amounts of Pesticides in Water and Food USI  
PI: Jenkins, co-PI: **Schneider** 07/27/2012 - 06/30/2013  
National Institute of Health, NIEHS/SBIR Phase II/R44  
(OSU subcontract through Dahl Natural Inc., PI: Schwartz) \$283,000
4. ONAMI: Intermolecular energy transfer: from exciton diffusion at nanoscale to low-threshold solid-state organic lasers  
PI: Ostroverkhova, co-PI: **Schneider** 1/1/2011 - 12/31/2011  
Office of Naval Research \$93,018

5. ONAMI: Nonlinear terahertz electrodynamics in graphene  
 PI: Lee, co-PIs: Minot, **Schneider** 1/1/2011 - 12/31/2011  
 Office of Naval Research \$180,708
6. BMACC: Blended, Multimodal Access to Computational Physics Curricula  
 PI: Landau, co-PI: **Schneider** 9/1/2009 - 8/31/2011  
 National Science Foundation \$148,569
7. Theory of High Efficiency Photovoltaics Utilizing Heterojunction-Assisted Impact Ionization  
 PI: **Schneider** 1/1/2010 - 12/31/2010  
 Research Office, Oregon State University, General Reserve Fund \$7,569
8. ONAMI: Electronic sensing of single molecule dynamics  
 PI: Minot, co-PIs: **Schneider**, Roundy, Fifield, Chapman 1/1/2009 - 12/31/2009  
 Office of Naval Research \$229,736
9. ONAMI: Identification, imaging and manipulation of charged states in organic semiconductors: from macroscopic to microscopic optoelectronic devices  
 PI: Ostroverkhova, co-PI: **Schneider** 1/1/2008 - 12/31/2008  
 Office of Naval Research \$102,632  
 Schneider component: \$15,000
10. High Performance Computing Cluster for Advanced Simulations in Materials Science and Nanotechnology  
 PI: **Schneider** 1/1/2007 - 12/31/2007  
 Research Office, Oregon State University, Research Equipment Reserve Fund \$37,676

### Service to Profession

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1. Conference Co-organizer: 384-th WE-Heraeus-Seminar, 1/30/2007-2/2/2007, Bad Honnef, Germany: *Nonequilibrium Transport of Strongly Correlated Systems*.
2. Technical program co-chair for IEEE Nano 2011 conference, 8/15-8/19/2011, Portland, OR.
3. Invited reviewer for grants submitted to National Science Foundation: Division of Materials Research, Theory Section. (2010-present)
4. Invited reviewer for peer-reviewed journals and refereed conference proceedings: Nature, Physical Review B, Journal of Applied Physics, and Nanotechnology. 15 reviews in 2011-2013.
5. Invited panel reviewer for Department of Energy: INCITE program. (2013)

### Awards

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1. Scholarship, Baden Württemberg - Oregon Universities Exchange Program (1992)
2. Fulbright Scholar Travel Grant (1992)