Patrick K. Schelling
Curriculum Vitae

Professional Preparation

University of Minnesota, Minneapolis, MN	Ph.D. 1999		Physics
University of Minnesota, Minneapolis, MN	B.S	1992	Physics

Appointments

5/09-present	Associate Professor, Department of Physics, U. of Central Florida, Orlando, FL
8/03-5/09:	Assistant Professor, Department of Physics, U. of Central Florida, Orlando, FL
5/01-7/03:	Visiting Scientist, Materials Science Division, Argonne National Laboratory, Argonne IL and Institute for Nanotechnology, Karlsruhe Germany
8/99-5/01:	Postdoctoral Researcher, Materials Science Division, Argonne NationalLaboratory, Argonne IL (advisers Simon Phillpot, Dieter Wolf)
8/95-8/99:	Graduate Research Assistant, Physics Department, University of Minnesota, Minneapolis MN (adviser J. Woods Halley)

Refereed Journal Articles:

1. P. K. Schelling, "Physical mechanism of the Soret effect in binary Lennard-Jones liquids elucidated with thermal-response calculations," *J. Chem Phys*. **158**, 044501 (2023) doi.org/10.1063/5.0135244
2. N. Bohm and P. K. Schelling, "Analysis of ballistic resonance in the α-Fermi-Pasta-Ulam-Tsinguo model," *Phys. Rev. E* **106**, 024212 (2022) doi.org/10.1103/PhysRevE.106.024212
3. B. D. Doan and P. K. Schelling, "Dissipation and adhesion hysteresis between (010) forsterite surfaces using molecular-dynamics simulation and the Jarzynski equality," *Comp. Mat. Sci*. **206**, 111259 (2022) doi.org/10.1016/j.commatsci.2022.111259
4. W. E. Richardson, E. R. Mucciolo, and P. K. Schelling, "Resistivity size effect due to surface steps on ruthenium thin films computed with a realistic tight-binding model," *Journal of Applied Physics* **130**, 195108 (2021) doi.org/10.1063/5.0069046
5. B. Doan, A. R. Dove, and P. K. Schelling, "Dissipation and adhesion between amorphous FeO nanoparticles," *J. Aero. Sci*. **155**, 105742 (2021) doi.org/10.1016/j.jaerosci.2020.105742
6. K. Barmak, S. Ezzat, R. Gusley, A. Jog, S. Kerdsongpanya, A. Khanya, E. Milosevic, W. Richardson, K. Sentosun, A. Zangiabadi, D. Gall, W. E. Kaden, E. R. Mucciolo, P. K. Schelling, A. C. West, and K. R. Coffey, "Epitaxial metals for interconnects beyond Cu", *J. Vac. Sci. Tech. A* **38**, 033406 (2020) doi.org/10.1116/6.0000018
7. K. Fernando and P. K. Schelling, "Non-local linear-response functions for thermal transport computed with equilibrium molecular-dynamics simulation," *J. Appl. Phys*. **128**, 215105 (2020) doi.org/10.1063/5.0032014

8. W. C. Tucker, A. R. Dove, and P. K. Schelling, "Dissipation and plastic deformation in collisions between metallic nanoparticles," *Comp. Mat. Sci.* **161**, 215-222 (2019) doi.org/10.1016/j.commatsci.2019.02.004
9. A. H. Quadery, B. Doan, W. C. Tucker, A. Dove, and P. K. Schelling, "Role of surface chemistry in grain adhesion and dissipation during collisions of silica nanograins," *The Astrophysical Journal* **84**, 105 (2017) doi.org/10.3847/1538-4357/aa7890
10. W. C. Tucker, A. H. Quadery, P. K. Schelling, A. Schulte, R. Blair, W. Kaden, and D. Britt, "Strong catalytic activity of iron nanoparticles on the surfaces of reduced olivine," *Icarus* **299**, 502-512 (2018) doi.org/10.1016/j.icarus.2017.08.027
11. W. C. Tucker and P. K. Schelling, "Thermodiffusion in liquid binary alloys computed from molecular-dynamics simulation and the Green-Kubo formalism," *Comp. Mat. Sci.* **124**, 54-61 (2016) doi.org/10.1016/j.commatsci.2016.07.012
12. Abrar Quadery, Shaun Pacheco, Alan Au, Natalie Rizzacasa, Joshua Nichols, Timothy Le, Cameron Glasscock, and Patrick K. Schelling, "Atomic-scale simulation of radiation damage in olivine and orthopyroxene," *J. Geophys. Res. Planets* **120,** 643-661 (2015) doi.org/10.1002/2014JE004683
13. W. C. Tucker and P. K. Schelling, "Analysis of simulation methodology for calculation of the heat of transport for vacancy thermodiffusion," *J. Appl. Phys.* **116**, 023504 (2014) doi.org/10.1063/1.4887121
14. P. K. Schelling, J. Ernotte, W. C. Tucker, J. W. Halley, and L. Shokeen, "Molecular-dynamics calculation of the vacancy heat of transport," *J. Appl. Phys.* **116**, 023506 (2014) doi.org/10.1063/1.4886577
15. D. Choi, X. Liu, P. K. Schelling, K. R. Coffey, and K. Barmak, "Failure of Theoretical Models to Describe Resistivity of Nanometric, Polycrystalline Tungsten Films," *J. Appl. Physics,* **115**, 104308 (2014) doi.org/10.1063/1.4868093
16. W. C. Tucker, L. Shokeen, and P. K. Schelling, "Atomic-scale simulation of the thermodiffusion of hydrogen in palladium," *J. Appl. Phys.* **114**, 063509 (2013) doi.org/10.1063/1.4816961
17. M. Sheng, P. K. Schelling, and P. Keblinski, "Heat transfer mechanism across few-layer graphene by molecular dynamics", *Phys. Rev. B.* **88**, 045444 (2013)
18. L. Shokeen and P. K. Schelling, "Role of electronic-excitation effects in the melting and ablation of laser-excited silicon," *Comp. Mat. Sci.* **67**, 316 (2013)
19. P. K. Schelling and T. Le, "Computational methodology for analysis of the Soret effect in crystals: Application to hydrogen in palladium," *J. Appl. Phys.* **112**, 083516 (2012)
20. Y. Chen, A. Chernatynskiy, D. Brown, P. K. Schelling, E. Artacho, and S. R. Phillpot, "Critical assessment of classical potentials for $MgSiO_3$ perovskite with application to thermal conductivity calculations," *Phys. Earth Plan. Inter.* **210-211**, 75 (2012)
21. Z. McDargh and P. K. Schelling, "Molecular-dynamics approach for determining the vacancy heat of transport," *Comp. Mat. Sci.* **50**, 2363 (2011)
22. L. Shokeen and P. K. Schelling, "Thermodynamics and kinetics of silicon under conditions of strong electronic excitation," *J. Appl. Phys.* **109**, 073503 (2011)
23. L. Shokeen and P. K. Schelling, "An empirical potential for silicon under conditions of strong electronic excitation," *Appl. Phys. Lett.* **97**, 151907 (2010)
24. P. K. Schelling, "Thermal conductivity of A-site doped pyrochlore oxides studied by molecular-dynamics simulation," *Comp. Mat. Sci.* **48**, 336 (2010)

25. T. Watanabe, S.G. Srivilliputhur, P.K. Schelling, J.S. Tulenko, S.B. Sinnott, and S.R. Phillpot, "Thermal Transport in Off-stoichiometric Uranium Dioxide by Atomic Level Simulation," *J. Am. Ceram. Soc.* **92**, 850 (2009)
26. Ming Hu, P. Keblinski, and P.K. Schelling, "Kapitza conductance of silicon-amorphous polyethylene interfaces by molecular-dynamics simulation," *Phys. Rev. B* **79**, 104305 (2009)
27. X.W. Zhou, S. Aubry, R.E. Jones, A. Greenstein, and P.K. Schelling, "Towards More Accurate Molecular Dynamics Calculations of Thermal Conductivity. Case study: GaN Bulk Crystals," *Phys. Rev. B* **79**, 115201 (2009)
28. S. Aubry, C. Kimmer, A. Skye, and P.K. Schelling, "Comparison of theoretical and simulation-based predictions of grain-boundary Kapitza conductance in silicon," *Phys. Rev. B* **78**, 064112 (2008)
29. P.K. Schelling, "Phase diagram and kinetics of a new bond-order potential for silicon," *Comp. Mat. Sci.* **44**, 274 (2008)
30. T. Watanabe, S.B. Sinnott, J.S. Tulenko, R.W. Grimes, P.K. Schelling, and S.R. Phillpot, "Thermal Transport Properties of Uranium Dioxide by Molecular Dynamics Simulation," *J. Nucl. Mat.* **375**, 388 (2008)
31. M. Yao, T. Watanabe, P.K. Schelling. P. Keblinski, D.G. Cahill, and S.R. Phillpot, "Phonon-defect scattering in doped silicon by molecular-dynamics simulation," *J. Appl. Phys.* **104**, 024905 (2008)
32. A. Skye and P.K. Schelling, "Thermal resistivity of Si-Ge alloys by molecular-dynamics simulation," *J. Appl. Phys.* **103**, 113524 (2008)
33. T. Watanabe, B. Ni, P.K. Schelling, P. Keblinski, and S.R. Phillpot, "Thermal Conductance Across Grain Boundaries in Diamond from Molecular Dynamics Simulation," *J. Appl. Phys.* **102**, 063503 (2007)
34. S. Aubry, C. Kimmer, A. Skye, and P.K. Schelling, "Scattering of phonons from a high-energy grain boundary in silicon: Dependence on angle of incidence," *Phys. Rev. B* **75**, 144105 (2007)
35. S. Kumar and P.K Schelling, "Basis-set optimization for first-principles simulation of liquid water," *Int. J. of Quant. Phys.* **107**, 556 (2007)
36. S. Kumar and P.K. Schelling, "Density-functional theory study of water adsorption at reduced and stoichiometric ceria (111) surfaces," *J. Chem. Phys.* **125**, 204704 (2006)
37. A. Bodapati, P.K. Schelling, S.R. Phillpot, and P. Keblinski, "Vibrations and Thermal Transport in Nanocrystalline Silicon," *Phys. Rev. B* **74**, 245207 (2006)
38. B. Becker, P. K. Schelling, and S. R. Phillpot, "Interfacial Phonon Scattering in Semiconductor Nanowires by Molecular-Dynamics Simulation," *J. Appl. Phys.* **99**, 123715 (2006)
39. A. Bodapati, P.K. Schelling, S.R. Phillpot, and P. Keblinski, "Crossover in thermal transport mechanism in nanocrystalline silicon," *Appl. Phys. Lett.* **88**, 141908 (2006)
40. M. A. Angadi, T. Watanabe, A. Bodapati, X. Xiao, O. Auciello, J. A. Carlisle, J. A. Eastman, P. Keblinski, P. K. Schelling, and S. R. Phillpot, "Thermal Transport and grain-boundary conductance in ultrananocrystalline diamond thin films," *J. Appl. Phys.* **99**, 114301 (2006)
41. P. K. Schelling, L. Shi, and K. E. Goodson, "Managing Heat for Electronics," *Mat. Today* **8**, 30 (2005)

42. P. Keblinski and P. K. Schelling, "Comment on "Thermal Contraction of Carbon Fullerenes and Nanotubes", *Phys. Rev. Lett.* **94**, 209701 (2005)
43. S. R. Phillpot, P. K. Schelling, and P. Keblinski, "Interfacial thermal conductivity: Insights from atomic level simulation," *J. Mat. Sci.* **40**, 3143 (2005)
44. S. Sinha, P. K. Schelling. S. R. Phillpot, and K. E. Goodson, "Scattering of g-process longitudinal optical phonons at hotspots in silicon," *J. Appl. Phys.* **97**, 023702 (2005)
45. B. Becker, P. K. Schelling, and S. R. Phillpot, "Computational studies of nanoscale phonon transport and interfacial scattering", Phys. Stat. Sol. (c) **1**, 2955 (2004)
46. P. K. Schelling, S. R. Phillpot, and P. Keblinski, "Kapitza conductance and phonon scattering at grain boundaries by simulation," *J. Appl. Phys.* **95**, 6082 (2004)
47. P. K. Schelling, S. R. Phillpot, and R. W. Grimes, "Optimum pyrochlore composition for low thermal conductivity by simulation," *Phil. Mag. Lett.* **84**, 127 (2004)
48. S. Sinha, P. K. Schelling, S. R. Phillpot, and K. E. Goodson, "Nanoscale simulation of heat conduction in semiconductor devices," ITHERM 2004 2, 734 (2004)
49. P. K. Schelling and P. Keblinski, "Thermal expansion of carbon structures," *Phys. Rev. B* **68**, 035425 (2003)
50. P. K. Schelling and S. R. Phillpot, "Multiscale simulation of phonon transport in superlattices," *J. Appl. Phys.* 93, 5277 (2003)
51. B. T. Cong, P. N. A. Huy, P. K. Schelling, and J. W. Halley, "Total energy calculation of perovskite $BaTiO_3$ by self-consistent tight-binding method," *Bull. Mat. Sci.* 26, 155 (2003)
52. P. K. Schelling, S. R. Phillpot, and P. Keblinski, "Phonon wave-packet dynamics at semiconductor interfaces by molecular-dynamics simulation," *Appl. Phys. Lett.* **80**, 2484 (2002)
53. P. K. Schelling, S. R. Phillpot, and P. Keblinski, "Comparison of atomic-level simulation methods for computing thermal conductivity," *Phys. Rev. B* **65**, 144306 (2002)
54. P. K. Schelling and S. R. Phillpot, "Mechanism of thermal transport in zirconia and yttria-stabilized zirconia by molecular-dynamics simulation," *J. Am. Cer. Soc.* **84**, 2997 (2001)
55. P. K. Schelling and J. W. Halley, "Analysis of photoluminescence experiments on p-type GaAs electrodes using a drift-diffusion model," *Phys. Rev. B* **64**, 04326 (2001)
56. P. K. Schelling, S. R. Phillpot, and D. Wolf, "Mechanism of the cubic-to-tetragonal phase transition in zirconia and yttria-stabilized zirconia by molecular-dynamics simulation," *J. Am. Cer. Soc.* **84**, 1609 (2001)
57. P. K. Schelling and J. W. Halley, "Localization of polarons: a calculation in the adiabatic approximation," *Phys. Rev. B* **62,** 3241 (2000)
58. J. W. Halley, P. K. Schelling, and Y. Duan, "Simulation methods for chemically specific modeling of electrochemical interfaces," *Electrochim. Acta* **46**, 239 (2000)
59. P. K. Schelling, N. Yu, and J. W. Halley, "Self-consistent tight-binding atomic-relaxation model of titanium dioxide," *Phys. Rev. B* **58**, 1279 (1998)

Peer-reviewed conference proceedings:

1. P. K. Schelling and J. W. Halley, "Modeling of semiconductor/electrolyte interfaces with tight-binding molecular dynamics," in *Solid-Liquid Interface Theory,* ACS Symposium Series **789**, ed. J. Woods Halley (2001)

2. R. W. Grimes, M. Pirzada, P.K. Schelling, S. R. Phillpot, K. E. Sickafus, and J. Maguire "Atomic Scale Simulations for Compositional Optimization," The 4th International Conference on Intelligent Processing and Manufacturing of Materials (2003)
3. M. Yao, T. Watanabe, S.R. Phillpot, P.K. Schelling, P. Keblinski, and D.G. Cahill, "Phonon Scattering in Doped Silicon by Molecular Dynamics Simulation," Nanotech 2006 Vol. 1, 677 (2006)

Invited presentations:

1. P. K. Schelling, K. R. Coffey, and K. Barmak, "Resistivity of oriented, single-crystal nanowires for interconnects: A theoretical investigation," IPS Back-End Processes and Packing Review, Semiconductor Research Corporation (SRC), June 18-20 (2013), Georgia Tech
2. P. K. Schelling and A. Quadery, "Opportunities for the application of atomic-scale simulation to elucidate space-weathering processes," (2013), SRI grantee workshop, University of Florida
3. P. K. Schelling "Atomic-scale modeling of laser-solid interactions including electronic excitations," International High-Power Laser Ablation and Beamed Energy Propulsion, April 21-25, 2014 Santa Fe, New Mexico
4. P. K. Schelling, "Opportunities for the Application of Atomic-Scale Simulation to Elucidate the Space Weathering Process," 1st Space Research Institute Annual Workshop, Florida Space Institute, November 14, 2013
5. P. K. Schelling, "Opportunities for the Application of Atomic-Scale Simulation to Elucidate the Space Weathering Process," Florida Space Institute Seminar, April 10, 2013
6. P. K. Schelling and L. Shokeen, "Modeling Silicon Excited by Femtosecond Laser Pulses**"** MRS Spring Meeting, April 2011
7. P.K. Schelling, A. Skye, S. Aubry, and C. Kimmer, "Theory and simulation of phonon transport in bulk and interfacial systems," Florida Society for Materials Simulation, annual meeting, Florida State University, May 2008
8. P.K. Schelling, A. Skye, S. Aubry, and C. Kimmer, "Theory and simulation of phonon transport in bulk and interfacial systems," Florida AVS meeting, University of Central Florida, May 2008
9. P. K. Schelling, A. Skye, J. Blandon, A. Greenstein, T. Watanabe, S.R. Phillpot, S. Aubry, and C. Kimmer, "Phonon and thermal transport in nanocrystalline materials," Sandia National Labs, Livermore CA, August 2007
10. P.K. Schelling, A. Skye, S.R. Phillpot, C. Kimmer, E. Piekos, and Sylvie Aubry, "Dynamics and thermal transport in the nanoscale regime," Florida Society for Materials Simulation, University of S. Florida, June 2007
11. P.K. Schelling, A. Skye, S. Aubry, and C. Kimmer, "Dynamics and thermal transport in the nanoscale regime," 9th US Congress Comp. Mech., San Francisco CA, July 2007
12. P.K. Schelling and B.Becker, "Nanoscale thermal transport studied using wave-packet dynamics," Sandia National Laboratory, August 2006

13. P.K. Schelling, B. Becker, S.R. Phillpot, A. Bodapati, P. Keblinski, C. Kimmer, E. Piekos, S. Aubry, "Dynamics and thermal transport in the nanoscale regime," Materials Science and Engineering Department, Rensselaer Polytechnic Institute, June 2006
14. P.K Schelling and S. Kumar, "Electronic-structure methods applied to problems in catalysis and electrochemistry," Florida Society for Materials Simulation, annual meeting, University of Central Florida, May 2006
15. P.K. Schelling, B. Becker, S.R. Phillpot, and C. Kimmer, "Phonon transport and scattering using molecular dynamics simulation," Sandia National Laboratory, Livermore CA, June 2005
16. P.K. Schelling, S. Kumar, and J.W. Halley, "Electronic-structure simulation for large-scale systems including oxides, metals, and nanoparticles," University of Florida, Department of Materials Science and Engineering, April 2005
17. P.K. Schelling, B. Becker, and S.R. Phillpot, "Simulation of phonon transport in semiconductor nanostructures," Florida Society for Materials Simulation, annual meeting, University of Florida, August 2005
18. P.K. Schelling, B. Becker, S.R. Phillpot, and P. Keblinski, "Simulation studies of interface and surface properties in phonon-mediated thermal transport," TMS Annual Meeting, San Francisco, CA February 2005
19. P.K. Schelling and S.R. Phillpot, "Multiscale Simulation of Thermal Transport in Nanostructures," MRS Spring Meeting, April 2003
20. P.K. Schelling, "Multiscale simulation of thermal transport and phonon dynamics," University of California at Irvine, Materials Science Department, April 2003
21. P.K. Schelling, "Multiscale simulation of thermal transport and phonon dynamics," University of Michigan, Mechanical Engineering Department, April 2003
22. P.K. Schelling, "Multiscale simulation of thermal transport and phonon dynamics," University of Central Florida, Department of Physics. April 2003
23. P.K. Schelling and S.R. Phillpot, "Multiscale Simulation of Thermal Transport in Nanostructures," MRS Spring Meeting, April 2003
24. P. K. Schelling and J. W. Halley, "Modeling of semiconductor/electrolyte interfaces with tight-binding molecular dynamics," American Chemical Society, New Orleans, LA 1999
25. P.K. Schelling and S.R. Phillpot, "Multiscale Simulation of Thermal Transport and Phonon Dynamics," American Ceramics Society, St. Louis, MO April 2002

Contributed presentations:

1. **P. K. Schelling**, D.T. Britt, A. H. Quadery, W. C. Tucker, and R. Blair, "*Atomic-Scale Modeling and Theory of Space Weathering Processes: Mechanisms and Surface Properties,*" Workshop of Space Weathering of Airless Bodies, Nov. 2-4, 2015 Houston, TX
2. **D. T. Britt**, P. K Schelling, and R. Blair, "*The Chemistry and Physics of Space Weathering,"* Workshop of Space Weathering of Airless Bodies, Nov. 2-4, 2015 Houston, TX

3. **R. Blair,** P. K. Schelling, and D. T. Britt, "*Aspects of Space Weathering via Mechanically Initiated Chemistry,"* Workshop of Space Weathering of Airless Bodies, Nov. 2-4, 2015 Houston, TX
4. P. K. Schelling**,** D. T. Britt, T. Bradley, and G. J. Consolmagno, "Space Weathering on Mercury and Vesta," 45th Lunar and Planetary Science Conference, p. 2179, March 17-21, 2014 Woodlands Texas, Contributed, International
5. D. T. Britt**,** P. K. Schelling, G. J. Consolmagno, and T. Bradley, "Space Weathering on Volatile-Rich Asteroids," 45th Lunar and Planetary Science Conference, p. 2179, March 17-21, 2014 Woodlands Texas, Contributed, International
6. P. K. Schelling, S.R. Phillpot, and D. Wolf, "Grain-boundary effects on thermal conductivity in yttria-stabilized zirconia by molecular dynamics," MRS Symposium, Boston MA, Fall 2000
7. M. Zhuang, J.W. Halley, and P.K. Schelling, "Self-consistent tight-binding description of thin oxide films on metals," MRS Symposium, Boston MA, Fall 2001
8. S. Sinha, P.K. Schelling, S.R. Phillpot, K. Goodson, "Atomic simulation of phonon hotspots in silicon devices," MRS Symposium, San Francisco CA, Spring 2003
9. R.W. Grimes, M. Pirzada, P.K. Schelling, S. R. Phillpot, K. E. Sickafus, and J. Maguire "Atomic Scale Simulations for Compositional Optimization," The 4th International Conference on Intelligent Processing and Manufacturing of Materials 2003
10. P.K. Schelling, B. Becker, S.R. Phillpot, and P. Keblinksi, "Phonon wave-packet scattering at semiconductor interfaces," Phonons2004 international meeting, St. Petersburg Russia, 2004
11. A. Bodapati, P. Keblinski, and P. K. Schelling, "Thermal transport in nanocrystalline silicon," MRS Symposium, San Francisco CA, Spring 2005
12. S.R. Phillpot, T. Watanabe, P.K. Schelling. P. Keblinski, "Interfacial thermal transport: Insights from simulation," MRS Symposium, San Francisco CA, Spring 2005
13. A. Bodapati, P. Keblinski, and P.K. Schelling, "Phonon dynamics in carbon nanotubes," MRS Symposium, San Francisco CA, Spring 2005
14. M. Yao, T. Watanabe, S.R. Phillpot, P.K. Schelling, P. Keblinski, and D.G. Cahill, "Phonon scattering and thermal conductivity in doped silicon by molecular dynamics simulation," NSTI Nanotech Boston MA 2005
15. P.K. Schelling, B. Becker, and S.R. Phillpot, "Phonon transport and scattering in semiconductor nanowires," MRS Symposium, San Francisco CA, Spring 2005
16. A. Bodapati, P. Keblinski, and P.K. Schelling, "Phonon dynamics in carbon nanotubes," APS meeting, Baltimore MD, 2006
17. S. Aubry, C. Kimmer, P.K. Schelling, and A. Skye "Thermal transport in silicon microsystems," 9th US Congress Comp. Mech., San Francisco CA, July 2007
18. S. Aubry, C. Kimmer, P.K. Schelling, E. Piekos, and L. Phinney, "Atomic scale modeling of phonon-mediated thermal transport in Microsystems," MRS Symposium, San Francisco CA, Spring 2007
19. P.K. Schelling, Y. Lin, N. Van Duc, S. Kumar, and J.W. Halley, "Kinetics of water adsorption at anatase nanoparticles," TMS Symposium, Orlando FL, Spring 2007

20. P.K. Schelling and L. Shokeen, "Electronic Excitation Effects in Laser Melting and Ablation of Silicon", MRS Fall Meeting, Boston, MA Fall 2012

Research grants:

1. UCF Presidential Equipment Initiative, PI Schelling, $36,400 (2004)
2. UCF In-House Award, PI Schelling, $7,500 (2004)
3. "US-Vietnam Cooperative Research in Computational Materials and Device Physics," NSF, PI R. Joynt (U. Wisconsin), coPI P.K. Schelling, J.W. Halley, and M. Friesen, $56,700
4. LDRD Sandia National Laboratory, Consultant, $21,000, 2005-6
5. "SFTI Ph1: Failure Mechanisms, Life Prediction and Enhanced Performance of Thermal and Environmental Barrier Coatings", PI Sohn, coPIs Schelling, An, Zhai, UCF-NASA-Glenn, 2/1/2007-3/31/2008, $170,000, $34,000 for Schelling
6. "Multiscale Simulation of Phonon Transport in Polycrystalline Silicon," Sandia National Laboratory, PI Schelling $10,500, 6/04/07-9/30/07
7. "NSF-REU in Computational Materials Science: Designing Materials in a Virtual Laboratory", PI A. Asthagiri (U. Florida), coPI P. Schelling, I. Oleynik, and A. El-Azab, $302,400, $75,600 for Schelling, 9/1/2008-9/31/2011
8. "Multiscale simulation of laser processing and ablation of semiconductor materials," PI Schelling, NSF-Materials Theory, $150,000 9/1/2008-9/31/2011
9. PI Schelling, coPI Yongho Sohn, "Multiscale Simulation and Experimental Study of Thermotransport in Binary Alloys," National Science Foundation, $390,000, 8/15/2011-8/14/2014
10. PI Schelling, coPIs Kevin Coffey and Katayun Barmak, "Resistivity of oriented, single-crystal nanowires for interconnects: A theoretical investigation," Semiconductor Research Corporation, $40,000 9/1/2012-8/31/2013
11. PI Schelling, "Opportunities for the Application of Atomic-Scale Simulation to Elucidate the Space Weathering Process" Florida Space Institute, $35,000, 1/1/2013-12/13/2013
12. PI Dan Britt, coPIs Schelling, Sohn, Bradley, "SRI: Catalyzed production of organic molecules on the surfaces of asteroids" $48,000 8/15/2013-7/31/2014
13. PI Schelling, coPI Dove, "Chemical and dynamical forces in building large particles in the disks around young stars, " National Science Foundation (Astronomy), $382K (50% credit) 2016-2020.
14. PI Coffey, coPI Schelling, Mucciolo, Kaden, Jiang, E2CDA: Collaborative Research: Type I: Interconnects beyond Cu," NSF/SRC $113K (Year 1 funding) (20% credit) (2017-2021)
15. PI Coffey, coPI Schelling, Kaden, and Mucciolo, "Thermoelectric phenomena in quasi one-dimensional metals," $252K (25% credit), Columbia University (AFOSR) (2018-2020) (Pending but expected to be approved)

Courses taught:

Undergraduate, introductory:

1. PHZ 3113, Introduction to theoretical methods, Spring 2004, 2005, 2010, 2011, 2012, 2014
2. PHY 2048, Physics for scientists and engineering, Fall 2012
3. PHY 2049, Physics for scientists and engineers, Fall 2004
4. PHY 2049H, Physics for scientists and engineers (honors), Spring 2007
5. PHY 2054, Introductory physics, Spring 2011, Fall 2011

Undergraduate, advanced:

6. PHY 4604, Wave mechanics I, Fall 2005
7. PHY 4605, Wave mechanics II, Spring 2006
8. PHY 3513, Thermal and Statistical Physics, Fall 2015, 2016
9. PHZ 3422, Nanophysics
10. PHZ 3466 Nanoscience III: Virtual Laboratory, Spring 2016, Fall 2017
11. PHY 3220 Mechanics I, Spring 2017, Sprint 2018
12. PHY 3513 Thermal and Statistical Physics

Graduate:

13. PHZ 5156, Computational physics, Fall 2006, 2007, 2011, 2013
14. PHY 5606, Quantum mechanics I, Spring 2008

Graduate students advised:

1. Santosh Kumar (AMPAC and MMAE), "Density-Functional Theory Applied to Problems in Catalysis and Electrochemistry", **graduated M.S. in Materials Science, July 2006**. Graduated with PhD in materials science from Purdue University, 2010
2. Ashton Skye (AMPAC and Physics), "Phonon-Mediated Thermal Transport in Silicon Nanowires by Molecular-Dynamics Simulation", **left before graduating**
3. Mark Nurge (Physics), "Electrical Capacitance Volume Tomography of High Contrast Dielectrics Using a Cuboid Geometry," **graduated with Ph.D. degree Spring 2007**
4. Duc Nguyen (Physics), **left for university in Netherlands, Fall 2008**
5. Dat Nguyen (Physics), **left to work in CREOL group, Spring 2007**
6. Lalit Shokeen (AMPAC and MSE), **PhD 2012,** employed at Global Foundaries
7. Abrar Quadery (Physics), **graduated PhD Fall 2017**
8. William (BJ) Tucker (Physics), **current student expected graduation Fall 2018**
9. Baochi Doan (MSE), PhD 2021
10. William Richardson (Physics) current

Graduate students co-advised:

1. A. Bodapati, "Structural Disorder and Thermal Transport in Nanoscale Solids," **graduated Ph.D. materials science Summer 2006**, Rensselaer Polytechnic Institute, advisor Pawel Keblinski
2. A. Greenstein, "Analysis of thermal conductivity models with an extension to complex crystalline materials," **graduated Ph.D. mechanical engineering Summer 2008**, Georgia Institute of Technology, adviser S. Graham

Undergraduate students advised:

1. Enrique Ortiz (Computer Science), RAMP fellowship student, "Electronic-structure based studies of adsorption and reaction of gas-phase molecules at gold nanoparticles," Fall 2005, Spring 2006
2. Nushien Shahnami (Physics), "Anharmonic scattering of phonons at grain boundary interfaces," Spring 2006
3. Tom Gordon (Physics), "Electronic-structure of semiconductor nanowires," Spring 2006
4. John Turpish (Physics), "Ionic transport and the Soret effect in yttria-stabilized zirconia," Summer 2007
5. Don Green (Physics), "Phonon transport in semiconductor nanowires," 2006
6. Tyler Gomez (Physics)
7. Dan Brown
8. Zachary McDargh
9. Shaun Pacheco
10. Alan Au
11. Josh Nichols
12. Natalie Rizzacasa
13. Jacques Ernotte
14. William Tucker
15. Timothy Le
16. Robert DeWitt
17. Nicholas Engman

Service activities:

Cluster lead (with Talat Rahman)
FCI: Energy Conversion and Propulsion

Interviewed and participated in hiring process for 3 faculty members (2 in Physics, 1 in Chemistry), with 2 additional offers for MSE and Env. Eng.

Professional society meeting chair and organization:

1. Session chair, TMS National Meeting, San Francisco CA, February 2005
2. Session Chair, MRS National Meeting, San Francisco CA, April 2005
3. Organized Florida Society for Materials Simulation Meeting and Workshop, UCF, May 2006
4. Cofounder and first president of the Florida Society for Materials Simulation, president 2006-7, 2010-11
5. Symposium organizer, "Nanoscale Thermal Transport: From Devices to Fundamentals," MRS National Meeting, San Francisco CA, April 2009
6. Symposium organizer, "Computational materials science," Florida AVS meeting, University of Central Florida, May 2008
7. Graduate student award judge, MRS symposium, Spring 2007

Other service, UCF meetings:

1. Undergraduate research poster judge, UCF SURE forum, 2007-11

Committee membership:

1. AMPAC space committee 2004
2. Physics undergraduate committee 2004-2006
3. Physics subcommittee for undergraduate textbooks, 2004, 2006
4. Physics qualifier exam committee 2005-2006
5. Physics subcommittee for graduate-student recruitment 2006-2007
6. Committee chair, graduate-student recruitment, 2007-present
7. IT committee, 2007-present
8. Physics colloquium committee, 2007-2008
9. Physics graduate admissions committee, member 2008, 2009, 2010-present, chair 2010-2011

Awards and honors:

Best Paper in Nanotechnology–Simulation, May (2003), The 4th International Conference on Intelligent Processing and Manufacturing of Materials, "Atomic Scale Simulations for Compositional Optimization," with R. W. Grimes, M. Pirzada, S. R. Phillpot, K. E. Sickafus, and J. Maguire

Ph.D. committees not as chair:

1. Juan Blandon, Ph.D. physics (Viatcheslava Kokoouline chair)
2. Jed Simmons, Ph.D. CREOL (Michael Bass chair)
3. Arun Bodapati, Ph.D. materials (RPI, Pawel Keblinski chair)
4. Luis Ono, Ph.D. physics (Beatriz Roldan-Cuenya chair)
5. Rashmi Mohanty, Ph.D. materials (Yongho Sohn chair)
6. Abe Greenstein, Ph.D. mechanical engineering, Georgia Inst. Tech. (Sam Graham chair)

Referee:

1. Proposal review, including NSF, DOE-BES, and ACS-Petroleum research fund
2. Journal review, including Phys. Rev. Lett., Phys. Rev. B, J. Appl. Phys., Appl. Phys. Lett., and J. Heat Trans.