Aleksandr V. Chernatynskiy

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Professional Appointments

2015-current: Assistant Professor, Department of Physics, Missouri University of Science and Technology.

2012-2015: Research Assistant Scientist, Department of Material Science and Engineering, University of Florida.

2008-2012: Postdoctoral Research Associate, Department of Material Science and Engineering, University of Florida (with Dr. Simon Phillpot).

2005-2008: Postdoctoral Research Associate, Physics Department, University of Minnesota (with Dr. Woods Halley).

Education

2001-2005: Ph.D. in Physical Chemistry, University of Louisville.

1999-2001: M.S. in Physics, University of Louisville.

1995-1999: B.S. in Theoretical Physics, Perm State University, Russia.

Awards

Research fellow at Minnesota Supercomputing Institute in University of Minnesota, 2006.
The Manuel Schwartz Award, Department of Physics, U of Louisville, 2006
N.V. Meshkov's Student Fellowship, Perm State University, Russia, 1997-1999

Funding

1. Co-PI on a project entitled: "Micro/Nano Scale AFM-based Thermal Conductivity Measurement and Atomistic Modeling for Oxide Fuel: the effects of grain boundary, fission gas and radiation damage", Idaho National Laboratory LDRD #13-105.

Publications

Accepted and Submitted Journal Articles

42. "*Nanoindentation of Gold and Gold Alloys by Molecular Dynamics Simulation*", Y. Li, A. Goyal, **A. Chernatynskiy**, J. S. Jayashankar, M. C. Kautzky, S. B. Sinnott, and S. R. Phillpot, submitted to PRB.
41. "*Systematic Investigation of the Misorientation- and Temperature-Dependent Kapitza Resistance in CeO_2*", **A. Chernatynskiy,** X.-M. Bai, J. Gan, submitted to Int. J. Heat Mass Transfer.
40. "*Seeing the invisible plasma with transient phonons in cuprous oxide*", L. Frazer, R. D. Schaller, K. B. Chang, **A. Chernatynskiy**, K. R. Poeppelmeier, submitted to Optic Lett.
39. "*Void nucleation in UO_2 by molecular dynamics simulation*", T.-W. Chiang, **A. Chernatynskiy**, S. B. Sinnott and S. R. Phillpot, Submitted to J. Nucl. Mater.

Published Journal Articles

38. *"Diffusion Across M/Pb(Zr,Ti)O_3 Interfaces (M=Pt_3Pb or Pt) as a Function of Pb Chemical Potential"*, F.-Y. Lin, **A. Chernatynskiy**, J. Nikkel, R. Bulanadi, J. L. Jones, J. C. Nino, S. B. Sinnott, J. Am. Cer. Soc., doi:10.1111/jace.13966.
37. *"Computational Discovery of Lanthanide Doped and Co-doped $Y_3Al_5O_{12}$ for Optoelectronic Applications"*, K. Choudhary, **A. Chernatynskiy**, K. Mathew, E. W. Bucholz , S. R. Phillpot, S. B. Sinnott, R. G. Hennig, Appl. Phys. Lett., 107, 112109 (2015), doi:10.1063/1.4929434.
36. *"Charge optimized many-body (COMB) potential for dynamical simulation of Ni–Al phases"*, A. Kumar, A. Chernatynskiy, Tao Liang, Kamal Choudhary, Mark J Noordhoek1, Yu-Ting Cheng2, Simon R Phillpot and Susan B Sinnott, J. Phys.: Cond. Matter. **27**, 336302 (2015), doi:10.1088/0953-8984/27/33/336302.
35. *"Combined experimental and computational methods reveal the evolution of buried interfaces during synthesis of ferroelectric thin films"*, J. L. Jones, J. M. LeBeau, J. Nikkel, A. A. Oni, J. H. Dycus, C. Cozzan, F.-Y. Lin, **A. Chernatynskiy**, J. C. Nino, S. B. Sinnott, S. Mhin, G. L. Brennecka, and J. Ihlefeld, Adv. Mater. Interfaces. **2** (2015), doi: 10.1002/admi.201500181
34. *"Anharmonic properties in Mg_2X (X=C, Si, Ge, Sn, Pb) from first-principles calculations"*, **A. Chernatynskiy** and S. R. Phillpot, Phys. Rev. B **92**, 064303 (2015), doi:10.1103/PhysRevB.92.064303.
33. *"Charge Optimized Many-Body (COMB) Potential for Al_2O_3 Materials, Interfaces, and Nanostructures"*, K. Choudhary, T. Liang, **A.Chernatynskiy**, S. R. Phillpot and S. Sinnott, J. Phys.: Cond. Matter. **27**, 305004 (2015), doi:10.1088/0953-8984/27/30/305004.
32. *"Phonon transport simulator (PhonTS)"*, **A. Chernatynskiy** and S. R. Phillpot, Comp. Phys. Comm., **192**, 196 (2015), doi:10.1016/j.cpc.2015.01.008.
31. *"Deformation Processes in Nanocrystalline Zr by Molecular Dynamics Simulations"* Z. Lu, M. J. Noordhoek, **A. Chernatynskiy**, S.B. Sinnott and S.R. Phillpot, J. Nucl. Mater., **462**, 147 (2015), doi:10.1016/j.jnucmat.2015.03.048.
30. *"An ab initio investigation of the effect of alloying elements on the elastic properties and magnetic behavior of Ni_3Al"* A. Kumar, **A. Chernatynskiy**, M. Hong, S.R. Phillpot and S.B. Sinnott, Comp. Mater. Sci. **101**, 39 (2015), doi:10.1016/j.commatsci.2015.01.007.
29. *"Charge Optimized Many-Body Potential for Aluminum"* K. Choudhary, T. Liang, **A. Chernatynskiy**, Z. Lu, A. Goyal, S.R. Phillpot and S.B. Sinnott, J. Phys.: Condens. Matter. **27**, 015003 (2015), doi:10.1088/0953-8984/27/1/015003.
28. *"Anisotropy in Oxidation of Zirconium Surfaces from Density Functional Theory Calculations"*, T.-W. Chiang, **A. Chernatynskiy**, M. J. Noordhoek, S. B. Sinnott and S. R. Phillpot, Comput. Mater. Sci. **98**, 112 (2015), doi:10.1016/j.commatsci.2014.10.052.
27. *"Effect of Pores and He Bubbles on the Thermal Transport Properties of UO_2 by Molecular Dynamics Simulation"*, C.-W. Lee, **A. Chernatynskiy**, P. Shukla, R. E. Stoller, S. B. Sinnott and S. R. Phillpot, J. Nucl. Mater. **456**, 253 (2015) doi:10.1016/j.jnucmat.2014.09.052.
26. *"A molecular dynamics study of tilt grain boundary resistance to slip and heat transfer in nanocrystalline silicon"*, X. Chen, L. Xiong, **A. Chernatynskiy** and Y. Chen, J. Appl. Phys. **116**, 244309 (2014) doi:10.1063/1.4905248.
25. *"Phonon thermal transport through tilt grain boundaries in strontium titanate"* Z. Zheng, X. Chen, B. Deng, **A. Chernatynskiy**, S. Yang, L. Xiong and Y. Chen, J. Appl. Phys. **116**, 073706 (2014) doi:10.1063/1.4893648.
24. *"Phonon Density of States and Anharmonicity of UO_2"*, J.W.L. Pang, **A. Chernatynskiy**, B. C. Larson, W.J.L. Buyers, D.L. Abernathy, K.J. McClellan, S.R. Phillpot, Phys. Rev. B **89**, 115132 (2014) doi:10.1103/PhysRevB.89.115132.

23. *"Kapitza resistance of Si/SiO_2 interface"*, B. Deng, **A. Chernatynskiy**, M. Khafizov, D. Hurley and S. R. Phillpot, J. Appl. Phys. **115**, 084910 (2014) doi:10.1063/1.4867047.
22. *"Interaction between Voids and Grain Boundaries in UO_2 by Molecular-Dynamics Simulation"*, T.-W. Chiang, **A. Chernatynskiy**, B. Deng, S. B. Sinnott and S. R. Phillpot, J. Nucl. Mater., **448**, 53 (2014) doi:10.1016/j.jnucmat.2014.01.027.
21. *"Thermal Conductivity in Nanocrystalline Ceria Thin Films"* M. Khafizov, I.-W. Park, **A. Chernatynskiy**, L. He, J. Lin, J.J. Moore, D. Swank, T. Lillo, S.R. Phillpot, A. El-Azab, D.H. Hurley, J. Am. Ceram. Soc. **97,** 562 (2014), doi: 10.1111/jace.12673.
20. *"Thermal conductivity of argon at high pressure from first principles calculations"* **A. Chernatynskiy** and S.R. Phillpot, J. App. Phys., **114**, 064902 (2013), doi:10.1063/1.4817901.
19. *"Uncertainty Quantification in Multiscale Simulation of Materials: A Prospective"*, **A. Chernatynskiy**, S. R. Phillpot and R. A. LeSar, Ann. Rev. Mater. Res., **43**, 157 (2013), doi:10.1146/annurev-matsci-071312-121708.
18. *"Phonon Lifetime Limited Thermal Conductivity of UO_2 by Neutron Scattering and Theory"* J. W.L. Pang, W. J.L. Buyers, **A. Chernatynskiy,** M. D. Lumsden, B. C. Larson and Simon R. Phillpot, Phys. Rev. Lett., **110**, 157401 (2013), doi:10.1103/PhysRevLett.110.157401.
17. *"Phonon-mediated Thermal Transport: Confronting Theory and Microscopic Simulation with Experiment"* **A. Chernatynskiy** and S. R. Phillpot, *Curr. Opin. Solid State Mater. Sci*, **17**, 1 (2013), doi:10.1016/j.cossms.2012.11.001.
16. *"Atomistic structure of (Ba,Sr)TiO_3: Comparing molecular-dynamics simulations with structural measurements"* M. J. Noordhoek, V. Krayzman, **A. Chernatynskiy**, S. R. Phillpot, and I. Levin, Appl. Phys. Lett., **103**, 022909 (2013), doi:10.1063/1.4813273.
15. *"Segregation of Ru to edge dislocations in UO_2"* A. Goyal, T. Rudzik, B. Deng, M. Hong, **A. Chernatynskiy**, S. B. Sinnott and S. R. Phillpot, J. Nucl. Mater., **441**, 96 (2013), doi:10.1016/j.jnucmat.2013.05.031.
14. *"Effects of Edge Dislocations on the Thermal Conductivity of UO_2"* B. Deng, **A. Chernatynskiy**, P. Shukla, S. Sinnott and S. R. Phillpot, J. Nucl. Mater., **434**, 203 (2013), doi:10.1016/j.jnucmat.2012.11.043.
13. *"Critical Assessment of Classical Potentials for $MgSiO_3$ Perovskite with Application to Thermal Conductivity Calculations"* Y. Chen, **A. Chernatynskiy**, P.K. Shelling, E. Artacho and S.R. Phillpot, Phys. Earth Planet. Inter., **210**, 75 (2012), doi:10.1016/j.pepi.2012.08.002.
12. *"Low Thermal Conductivity Oxides"* W. Pan, S. R. Phillpot, C. Wan, **A. Chernatynskiy** and Z. Qu, MRS Bull., **37**, 917 (2012), doi:10.1557/mrs.2012.234.
11. *"Critical assessment of UO_2 classical potentials for thermal conductivity calculations"* **A. Chernatynskiy,** C. Flint, S. Sinnott and S. R. Phillpot, J. Mater. Sci., **47**, 7693 (2012), doi:10.1007/s10853-011-6230-0.
10. *"Relativistic Tight-binding model: Application to Pt Surfaces"* **A. Tchernatinsky** and J. W. Halley, Phys. Rev. B, **83**, 205431 (2011), doi:10.1103/PhysRevB.83.205431.
9. *"Lattice Thermal Conductivity in Ionic Solids: Effects of Long Range Interactions"* **A. Chernatynskiy**, J. Turney, A. McGaughey, C.H. Amon and S.R. Phillpot. J. Am. Ceram. Soc., **94**, 3523 (2011), doi: 10.1111/j.1551-2916.2011.04743.x.
8. *"Thermal Conductivity of UO_2 Fuel: Predicting Fuel Performance from Simulation"* S. R. Phillpot, A. El-Azab, **A. Chernatynskiy** and J. S. Tulenko, JOM, **63**, 73-79 (2011), doi:10.1007/s11837-011-0143-x.
7. *"Effect of Inversion on Thermoelastic and Thermal-Transport Properties of $MgAl_2O_4$ and Related Spinels by Molecular-Dynamics Simulation"* P. Shukla, **A. Chernatynskiy**, J. C. Nino, S. B. Sinnott and S. R. Phillpot, J. Mater. Sci. **46,** 55 (2011), doi:10.1007/s10853-010-

4795-7.

6. *"Evaluation of Computational Techniques for Solving the Boltzmann Transport Equation for Lattice Thermal Conductivity Calculations"* **A. Chernatynskiy** and S.R. Phillpot, Phys. Rev. B, **82** 134301 (2010), doi:10.1103/PhysRevB.82.134301.
5. *"Stability and Charge Transfer Levels of Extrinsic Defects in $LiNbO_3$"*, H. Xu, **A. Chernatynskiy**, D. Lee, S. B. Sinnott, V. Gopalan, V. Dierolf, and S. R. Phillpot, Phys. Rev. B **82**, 184109 (2010), doi:10.1103/PhysRevB.82.184109.
4. "*Cross-over in Thermal Transport Properties of Natural, Perovskite-structured Superlattices"*, **A. Chernatynskiy**, R. W. Grimes, M. A. Zurbuchen, D. R. Clarke, and S. R. Phillpot, Appl. Phys. Lett. **95** 161906 (2009), doi:10.1063/1.3253421**.**
3. *"Anisotropic Thermal Properties in Orthorhombic Perovskite"*, B. Steele, A. D. Burns, **A. Chernatynskiy,** R. W. Grimes, and S. R. Phillpot, J. Mater. Sci., **45**, 168-176 (2010), doi:10.1007/s10853-009-3912-y.
2. *"Adsorption of Oxygen Molecules on Individual Carbon Single-walled Nanotubes"*, **A. Tchernatinsky,** B. Nagabhirava, S.Desai, G. Sumanasecera, B. Alphenaar, C.S. Jayanthi, and S.Y. Wu, J. Appl. Phys. **99**, 034306 (2006), doi:10.1063/1.2163008.
1. *"Spin System Radiofrequency Superradiation: a Phenomenological Study and comparison with Nimeric Simulation"*, C. L. Davis, V.K. Henner, **A. V. Tchernatinsky,** and I.V. Kaganov, Phys. Rev. B, **72**, 054406 (2005), doi:10.1103/PhysRevB.72.054406.

Book Chapters and Reports

2. *"Thermal Transport in Nanostructured Materials"* **A. Chernatynskiy**, D. R. Clarke and S. R. Phillpot, book chapter in "Handbook of Nanoscience, Engineering and Technology", 3rd Edition, CRC Press (2012).
1. *"Simulation of the Thermal Transport Properties of UO_2: Recent Progress and Current Challenges"* **A. Chernatynskiy**, A. El-Azab, J. Tulenko, S.R. Phillpot, to appear in "IAEA Review Report on Nuclear Fuels", 2014.

Software Development

1. PhonTS: Phonon transport simulator.
   A. Chernatynskiy and S.R. Phillpot, http://phonts.mse.ufl.edu

Professional Service

3. Reviewer of the research proposals for DOE, ARO and LLNL.
2. Referee for a manuscripts submitted to Physical Review Letters, Physical Reviews B, Journal of Applied Physics, and other journals.
1. Former Member of the Energy Frontiers Research Centers (EFRC) Newsletters editorial board, a publication devoted to popularization of the DOE EFRC program.

Invited Presentations

10. "*Evolution of voids in UO2 and their effect on thermal transport from atomic-resolution simulations*", T.-W. Chiang, C.-W. Lee, A. Chernatynskiy, S. B. Sinnott and S. R. Phillpot, MRS Spring Meeting, San Francisco, CA, 2015.
9. "*Thermal Conductivity: What Can We Learn from Atomistic Simulations*", A. Chernatynskiy, Seminar in Department of Mechanical Engineering, University of Florida. Jan, 2015.
8. "*Simulation of Complex Materials Structures with Charge Optimized Many-body (COMB) Potentials*", Y. Li, M. Noordhoek, T.-R. Shan, J. Martinez, A.

Chernatynskiy, T. Liang, S. B. Sinnott, S. Phillpot, MRS Spring Meeting, San Francisco, CA, 2014.

7. "*Thermal Transport at Extreme Environments from Atomistic Simulations*", A. Chernatynskiy, D. Bai, Y. Chen and S. Phillpot, MRS Fall Meeting, Boston, MA, November 2013.
6. "*Engineering Microstructure for Low Thermal Conductivity*", A. Chernatynskiy, S. Phillpot, MRS Spring Meeting, San-Francisco, CA, April 2013.
5. "*Understanding the Lattice Thermal Conductivity in Real Materials: Phonon-Phonon and Phonon-Defect Interactions from Atomistic Simulations*", A. Chernatynskiy, J. Pang, B. Deng, B. Larsen, W. Buyers and S. Phillpot, MRS Fall Meeting, Boston, MA, November 2011.
4. "*Thermal Conductivity and Lattice Dynamics"* invited seminar at Idaho National Lab.
3. *"Anisotropy of Thermal Transport in Solids"*, A. Chernatysnkiy and S. Phillpot, TSRC workshop on "Thermal Transport at Nanoscale", Telluride CO, June 2010.
2. *"Phonons Thermal Transport: Insights from Atomistic Simulations"* A. Chernatysnkiy and S. Phillpot; USC/DOE Conference "Emerging trends in materials simulations and experiments", Palos Verdes CA, 2010.
1. *"Relative Stability of Silicon Nanowires of Different Orientations"*. A. Tchernatinsky, C. Leahy, D. Migas, Y. Ming, C.S. Jayanthi, and S.Y. Wu., AIChE Annual Meeting, Cincinnati, 2005.

Teaching and Mentoring experience

2008-current: Mentored undergraduate students and visiting scholars in the research group that resulted in three published papers and two that are in preparation. Routinely substituted Dr. Phillpot in his "Molecular dynamics" class for a series of lectures on "Phonons"

2005-2008: Mentored students from Minnesota Supercomputing Institute summer REU program

2000-2005: Tutoring of courses of various levels in mathematics and physics.

1999-2000: Teaching assistantship in the Department of Physics, U of Louisville.

1995-1999: High school physics teacher in the School # 146, Perm, Russia.