Serge Nakhmanson

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Education

Ph.D. (Physics) Ohio University, Athens, OH. March 2001.
Dissertation: Theoretical studies of amorphous and paracrystalline silicon
Ph.D. advisor: D. A. Drabold

M.Sc. (Physics) St-Petersburg State University, St-Petersburg, Russia. December 1996.
Thesis: Paired states in homogeneous low-density electron gas
Thesis advisor: I. V. Abarenkov

B.S. (Physics) St-Petersburg State University, St-Petersburg, Russia. August 1994.

Employment

2013–present	Associate Professor (tenure track) Department of Materials Science & Engineering and Institute of Materials Science, University of Connecticut (Storrs)
2006–2012	Assistant Scientist Materials Science Division, Argonne National Laboratory
2004–2006	Postdoctoral Research Associate, Rutgers University *Postdoctoral advisors:* K. M. Rabe and D. Vanderbilt
2001–2004	Postdoctoral Research Associate, NC State University *Postdoctoral advisor:* J. Bernholc

Professional Accomplishments and Awards

Publications (see full list on pages 4–8)

56 papers in peer-reviewed journals: Science (1), Nature Mater. (1), NPJ Comp. Mater. (1), Rep. Prog. Phys. (1), Nanoscale (1), Phys. Rev. Lett. (4), Comput. Sci. Eng. (1), Appl. Phys. Lett. (4), Phys. Rev. B (19), etc.;
2 book chapters, 4 in conference proceedings;
1500+ lifetime citations, h-index = 19 (Google scholar, 8/20/2017).

Conferences (see full list on pages 8–17)

25 invited talks, 33 seminars, 70 contributed talks.

Awards

Honors Condensed Matter and Solid State Program stipend, Ohio University, 2000.

Professional Activities

2017–2018: *"Mesoscale phenomena in ferroic nanostructures: beyond the thin-film paradigm"* symposium organizer, MRS Fall Meeting 2018.

2017–2018: *"Mesoscale phenomena in ceramic materials"* symposium co-organizer, ACerS Conference on Electronic and Advanced Materials, Orlando FL, January 17–19, 2018.

2016–present: Director of Undergraduate Studies, Department of Materials Science & Engineering, University of Connecticut (Storrs).

2016–2017: *"Mesoscale phenomena in ceramic materials, nano- and microstructures"* symposium organizer, ACerS Electronic Materials and Applications Meeting, Orlando FL, January 18–20, 2017.

2016: *"Complex oxides"* symposium organizer, 5th International Conference from Nanoparticles and Nanomaterials to Nanodevices and Nanosystems (IC4N), Porto Heli, Greece, June 26–30, 2016.

2015–2016: *"Emerging functionalities in layered-oxide and related materials"* symposium organizer, ACerS Electronic Materials and Applications Meeting, Orlando FL, January 20–22, 2016.

2014–2015: *"Ceramic Composites, Coatings, and Fibers"* symposium co-organizer, ACerS Electronic Materials and Applications Meeting, Orlando FL, January 21–23, 2015.

2012–2013: *"Emergent Properties of Polar Interfaces and Nanostructures"* symposium organizer, IMRC Meeting, Cancun, Mexico, August 2013.

2011–2012: Chief organizer and session chair, Workshop on Fundamental Physics of Ferroelectrics and Related Materials at Argonne National Laboratory, Jan–Feb, 2012.

2011: Co-organizer of the Argonne Physical Sciences and Engineering directorate visit to the Thomas Young Centre for theory and simulation of materials, London UK, August 2011.

2010: Invited tutorial *"First principles calculations of polarization and phonons in ferroelectric materials with Quantum Espresso,"* for the International Symposium on Integrated Functionalities, San Juan PR, June 13–16, 2010.

2009–2010: *"Dielectric, Ferroelectric and Piezoelectric Oxides"* symposium organizer and session chair for the 2010 American Physical Society March meeting, Portland OR, March 15–19, 2010.

2009: *"Synthesis and characterization of ferroelectric materials: theory and experiment"* symposium organizer and session chair for the 21st International Symposium on Integrated Ferroelectrics and Functionalities, Colorado Springs CO, September 27–30, 2009.

- Proposal reviewer for the DoE and NSF.
- Reviewer for Phys. Rev. B, Phys. Rev. Lett., Appl. Phys. Lett., Nature Materials, J. Phys. Chem. Solids, etc.

Students and Postdocs (co)supervised

- 2016–present: Lukasz Kuna (Physics, UConn)
- 2016–present: Ayana Ghosh (MSE, UConn)
- 2014–2017: John Mangeri (Physics, UConn; PhD. degree awarded Aug 2017)
- 2013–present: Krishna C. Pitike (MSE, UConn)
- 2013–2017: Dr. Lydie Louis (IMS/MSE, UConn)
- 2012–2013: Dr. Shiyuan Gu (Mesoscale Elastic Problems LDRD, ANL)
- 2010–2012: Dr. William Parker (ALCF Computational Postdoctoral Fellow, ANL)
- 2007–2010: Dr. Rafal Korlacki (Molecular Ferroelectric Materials DoE-EPSCoR, University of Nebraska–Lincoln)
- 2007–2009: Dr. Jun He (ANL).

Society Memberships

1998–present: American Physical Society member

2013–present: American Ceramic Society member

2013–present: Materials Research Society member

Journal Articles and Book Chapters

[60] L. Louis, K. C. Pitike, S. Poddar, S. Ducharme, S. M. Nakhmanson, *Polarization canting in ferroelectric diisopropylammonium-halide molecular crystals: a computational first principles study,* submitted (2017).

[59] R. Agarwal, Y. Sharma, S. Chang, K. C. Pitike, C. Sohn, S. M. Nakhmanson, C. G. Takoudis, H. N. Lee, J. F. Scott, R. S. Katiyar, S. Hong, *Lead-free relaxor ferroelectricity and photovoltaic effects in $SnTiO_x$ directly deposited on Si substrate,* submitted (2017).

[58] L. Kuna, J. Mangeri, P.-X. Gao, S. Nakhmanson, *Stress-induced shift of band gap in ZnO nanowires from finite-element modeling,* in press, Phys. Rev. Applied (2017).

[57] S. F. Yuk, K. C. Pitike, S. M. Nakhmanson, M. Eisenbach, Y. W. Li, V. R. Cooper, *Towards an accurate description of perovskite ferroelectrics: exchange and correlation effects,* Sci. Rep. **7,** 43482 (2017).

[56] J. Mangeri, Y. Espinal, A. Jokisaari, S. P. Alpay, S. Nakhmanson, O. Heinonen, *Topological phase transformations and intrinsic size effects in ferroelectric nanoparticles,* Nanoscale **9,** 1616 (2017).

[55] A. Ghosh, T. Ahmed, D. A. Yarotski, S. M. Nakhmanson, J.-X. Zhu, *Oxygen vacancy effects on double perovskite Bi_2FeMnO_6: A first-principles study,* Europhys. Lett. **116,** 57002 (2016).

[54] T. Wang, K. C. Pitike, Y. Yuan, S. M. Nakhmanson, V. Gopalan, B. Jalan, *Chemistry, growth kinetics, and epitaxial stabilization of Sn^{2+} in Sn-doped $SrTiO_3$ using $(CH_3)_6Sn_2$ tin precursor,* APL Mater. **4,** 126111 (2016).

[53] J. Mangeri, K. C. Pitike, S. P. Alpay, S. M. Nakhmanson, *Amplitudon and Phason Modes of Electrocaloric Energy Interconversion,* NPJ Comp. Mater. **2**, 16020 (2016).

[52] S. Hong, S. M. Nakhmanson, D. D. Fong, *Screening mechanisms at polar oxide heterointerfaces,* Rep. Prog. Phys. **79**, 076501 (2016).

[51] S. Chang, S. K. Selvaraj, Y.-Y. Choi, S. Hong, S. M. Nakhmanson, and C. G. Takoudis, *Atomic layer deposition of environmentally benign $SnTiO_x$ as a potential ferroelectric material,* J. Vac. Sci. Technol. A **34**, 01A119 (2016).

[50] M. P. Cosgriff, P. Chen, S. S. Lee, H. J. Lee, L. Kuna, K. C. Pitike, L. Louis, W. D. Parker, H. Tajiri, S. M. Nakhmanson, J. Y. Jo, Z. Chen, L. Chen, and P. G. Evans, *Nanosecond Phase Transition Dynamics in Compressively Strained Epitaxial $BiFeO_3$,* Adv. Electron. Mater. **2**, 1500204 (2016).

[49] Y. Li, C. Adamo, P. Chen, P. G. Evans, S. M. Nakhmanson, W. Parker, C. E. Rowland, R. D. Schaller, D. G. Schlom, D. A. Walko, H. Wen, and Q. Zhang, *Giant optical enhancement of strain gradient in ferroelectric $BiFeO_3$ thin films and its physical origin,* Sci. Rep. **5,** 16650 (2015).

[48] F.-C. Sun, A. M. Dongare, A. D. Asandei, S. P. Alpay and S. Nakhmanson, *Temperature dependent structural, elastic, and polar properties of ferroelectric polyvinylidene*

fluoride (PVDF) and trifluoroethylene (TrFE) copolymers, J. Mater. Chem. C **3**, 8389–8396 (2015).

[47] J. Mangeri, O. Heinonen, D. Karpeyev, and S. Nakhmanson, *Influence of elastic and surface strains on the optical properties of semiconducting core-shell nanoparticles,* Phys. Rev. Applied **4**, 014001 (2015).

[46] L. Louis and S. M. Nakhmanson, *Structural, vibrational, and dielectric properties of Ruddlesden-Popper Ba_2ZrO_4 from first principles,* Phys. Rev. B **91**, 134103 (2015).

[45] K. C. Pitike, W. D. Parker, L. Louis, and S. M. Nakhmanson, *First-principles studies of lone-pair-induced distortions in epitaxial phases of perovskite $SnTiO_3$ and $PbTiO_3$,* Phys. Rev. B **91**, 035112 (2015).

[44] J. H. Lee, G. Luo, I. C. Tung, S. H. Chang, Z. Luo, M. Malshe, M. Gadre, A. Bhattacharya, S. M. Nakhmanson, J. A. Eastman, H. Hong, J. Jellinek, D. Morgan, D. D. Fong, and J. W. Freeland, *Dynamic layer rearrangement during growth of layered oxide films by molecular beam epitaxy,* Nature Mater. **13**, 879–883 (2014).

[43] B. Lee, S. M. Nakhmanson and O. Heinonen, *Strain induced vortex-to-uniform polarization transitions in soft-ferroelectric nanoparticles,* Appl. Phys. Lett. **104**, 262906 (2014).

[42] D. J. Li, S. Hong, S. Gu, Y. Choi, S. Nakhmanson, O. Heinonen, D. Karpeev, and K. No, *Polymer piezoelectric energy harvesters for low wind speed,* Appl. Phys. Lett. **104**, 012902 (2014).

[41] W. D. Parker and S. M. Nakhmanson, *Density functional study of the structural, electronic, and vibrational properties of β-Ba_2TiO_4,* Phys. Rev. B **88**, 245108 (2013).

[40] W. D. Parker and S. M. Nakhmanson, *Strain-induced incommensurate distortions in epitaxial Ruddlesden-Popper-type Ba_2TiO_4,* Phys. Rev. B **88**, 035203 (2013).

[39] J. He, G. B. Stephenson, S. M. Nakhmanson, *Electronic surface compensation of polarization in $PbTiO_3$ films,* J. Appl. Phys. **112**, 054112 (2012).

[38] V. Železný, A. Soukiassian, X. X. Xi, D. G. Schlom, J. Hlinka, C. Kadlec and S. M. Nakhmanson, *Infrared Spectroscopy of Nanoscopic Epitaxial $BaTiO_3/SrTiO_3$ Superlattices,* Integrated Ferroelectrics **134,** 146 (2012).

[37] P. Chen, J. Y. Jo, H. N. Lee, E. M. Dufresne, S. M. Nakhmanson, and P. G. Evans, *Domain- and symmetry-transition origins of reduced nanosecond piezoelectricity in ferroelectric/dielectric superlattices,* New J. Phys. **14**, 013034 (2012).

[36] W. D. Parker, J. M. Rondinelli, and S. M. Nakhmanson, *First-principles study of misfit strain-stabilized ferroelectric $SnTiO_3$,* Phys. Rev. B **84,** 245126 (2011).

[35] J. Hlinka, V. Železný, S. M. Nakhmanson, A. Soukiassian, X. X. Xi, and D. G. Schlom, *Soft-mode Spectroscopy of epitaxial $BaTiO_3/SrTiO_3$ Superlattices,* Phys. Rev. B **82,** 224102 (2010).

[34] J. Y. Jo, R. J. Sichel, E. M. Dufresne, H. N. Lee, S. M. Nakhmanson, and P. G. Evans, *Component-specific electromechanical response in a ferroelectric/dielectric superlattice,* Phys. Rev. B **82,** 174116 (2010).

[33] J. Y. Jo, R. J. Sichel, H. N. Lee, S. M. Nakhmanson, E. M. Dufresne, and P. G. Evans, *Piezoelectricity in the dielectric component of nanoscale dielectric/ferroelectric superlattices,* Phys. Rev. Lett. **104,** 207601 (2010).

[32] S. M. Nakhmanson, R. Korlacki, J. Travis Johnson, S. Ducharme, Z. Ge and J. M. Takacs, *Vibrational properties of ferroelectric β-vinylidene fluoride polymers and oligomers,* Phys. Rev. B **81,** 174120 (2010).

[31] V. Ranjan, L. Yu, S. Nakhmanson, J. Bernholc, M. Buongiorno Nardelli, *Polarization Effects and Phase Equilibria in High Energy Density PVDF-based Polymers,* Acta Cryst. A **66,** 553-557 (2010).

[30] S. M. Nakhmanson and I. Naumov, *Goldstone-like states in a layered perovskite with frustrated polarization: a first-principles investigation of $PbSr_2Ti_2O_7$,* Phys. Rev. Lett. **104,** 097601 (2010).

[29] S. M. Nakhmanson, *Revealing latent structural instabilities in perovskite ferroelectrics by layering and epitaxial strain: a first-principles study of Ruddlesden-Popper superlattices,* Phys. Rev. B **78,** 064107 (2008).

[28] D. A. Tenne, I. E. Gonenli, A. Soukiassian, D. G. Schlom, S. M. Nakhmanson, K. M. Rabe, X. X. Xi, *Raman study of oxygen reduced and re-oxidized strontium titanate,* Phys. Rev. B **76,** 024303 (2007).

[27] H. N. Lee, S. M. Nakhmanson, M. F. Chisholm, H. M. Christen, K. M. Rabe, and D. Vanderbilt, *Suppressed Dependence of Polarization on Epitaxial Strain in Highly Polar Ferroelectrics,* Phys. Rev. Lett. **98,** 217602 (2007).

[26] J. Bernholc, W. Lu, S. M. Nakhmanson, P. H. Hahn, V. Meunier, M. Buongiorno Nardelli, W. G. Schmidt, *Atomic scale design of nanostructures,* Mol. Phys. **105,** 147–156 (2007).

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[23] S. M. Nakhmanson, M. Buongiorno Nardelli, and J. Bernholc, *Collective polarization effects in β-polyvinylidene fluoride and its copolymers with tri- and tetrafluoroethylene,* Phys. Rev. B **72,** 115210 (2005).

[22] S. M. Nakhmanson, K. M. Rabe, and D. Vanderbilt, *Polarization enhancement in two- and three-component ferroelectric superlattices,* Appl. Phys. Lett. **87,** 102906 (2005).

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[20] J. Bernholc, S. M. Nakhmanson, M. Buongiorno Nardelli, and V. Meunier, *Understanding and enhancing polarization in complex materials,* Comput. Sci. Eng. **6,** 12–21 (2004).

[19] S. V. Khare, S. M. Nakhmanson, P. M. Voyles, P. Keblinski, and J. R. Abelson, *Evidence from simulations for orientational medium range order in fluctuation-electron-microscopy observations of a-Si,* Microsc. Microanal. **10** (Suppl 2), 820–821 (2004).

[18] S. V. Khare, S. M. Nakhmanson, P. M. Voyles, P. Keblinski, and J. R. Abelson, *Evidence from atomistic simulations of fluctuation electron microscopy for preferred local orientations in amorphous silicon,* Appl. Phys. Lett. **85,** 745–747 (2004).

[17] S. M. Nakhmanson, M. Buongiorno Nardelli and J. Bernholc, *Ab initio studies of polarization and piezoelectricity in vinylidene fluoride and BN-based polymers,* Phys. Rev. Lett. **92,** 115504 (2004).

[16] S. M. Nakhmanson, A. Calzolari, V. Meunier, J. Bernholc and M. Buongiorno Nardelli, *Spontaneous polarization and piezoelectricity in boron nitride nanotubes,* Phys. Rev. B **67,** 235406 (2003).

[15] J. Fabian, J. L. Feldman, C. Stephen Hellberg, and S. M. Nakhmanson, *Numerical study of anharmonic vibrational decay in amorphous and paracrystalline silicon,* Phys. Rev. B **67,** 224302 (2003).

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[13] S. M. Nakhmanson and N. Mousseau, *Crystallization study of model tetrahedral semiconductors,* J. Phys.: Condens. Matter **14,** 6627–6638 (2002).

[12] N. Mousseau, G. T. Barkema and S. M. Nakhmanson, *Recent developments in the study of continuous random networks,* Philos. Mag. B **82,** 171–183 (2002).

[11] S. Nakhmanson, N. Mousseau, G. T. Barkema, P. M. Voyles and D. A. Drabold, *Models of Paracrystalline Silicon with a Defect-Free Bandgap,* Intl. J. Mod. Phys. B **15** 3253–3257 (2001).

[10] P. M. Voyles, N. Zotov, S. M. Nakhmanson, D. A. Drabold, J. M. Gibson, M. M. J. Treacy, P. J. Keblinski, *Structure and Physical Properties of Paracrystalline Atomistic Models of Amorphous Silicon,* J. Appl. Phys. **90,** 4437–4451 (2001).

[9] S. Nakhmanson, P. M. Voyles, N. Mousseau, G. T. Barkema and D. A. Drabold, *Realistic Models of Paracrystalline Silicon,* Phys. Rev. B **63,** 235207 (2001).

[8] D. A. Drabold, S. Nakhmanson and X. Zhang, *Electronic structure of amorphous insulators and photostructural effects in chalcogenide glasses,* in *"Properties and Applications of Amorphous Materials,"* pp. 221–250, M. Thorpe and L. Tichy, Eds., Kluwer (2001).

[7] S. Nakhmanson and D. A. Drabold, *Low-temperature anomalous specific heat without tunneling modes: a simulation for a-Si with voids,* Phys. Rev. B **61,** 5376–5380 (2000).

[6] S. Nakhmanson and D. A. Drabold, *Computer simulation of low-energy excitations in amorphous silicon with voids,* J. Non-Cryst. Sol. **266–269,** 156–160 (2000).

[5] D. A. Drabold, U. Stephan, J. Dong and S. Nakhmanson, *Electronic structure of amorphous silicon,* J. Mol. Graphics Mod. **17,** 285–291, (1999).

[4] P. A. Fedders, D. A. Drabold and S. Nakhmanson, *Theoretical study on the nature of band-tail states in amorphous Si,* Phys. Rev. B **58,** 15624–15631 (1998).

[3] S. Nakhmanson and D. A. Drabold, *Approximate ab initio calculation of vibrational properties of hydrogenated amorphous silicon with inner voids,* Phys. Rev. B **58,** 15325–15328 (1998).

[2] S. A. Nemov, V. I. Proshin, S. M. Nakhmanson, *Effect of In doping on the kinetic coefficients in solid solutions of the system* $\left(Pb_zSn_{1-z}\right)_{0.95}Ge_{0.05}Te$*,* Semiconductors **32,** 1062–1064 (1998).

[1] S. M. Nakhmanson, A. Vashuta, I. V. Abarenkov, *Paired states in homogeneous low-density electron gas,* St-Petersburg State University Journal (1997) [in Russian].

Unrefereed conference proceedings:

[4] J. Bernholc, M. Buongiorno Nardelli, W. Lu, V. Meunier, S. M. Nakhmanson, and Q. Zhao, *Atomic scale design of nanostructures,* Proc. Indo-US workshop on *"Nanoscale Materials: From Science to Technology,"* pp. 145–154, S. N. Sahu, R. K. Choudhury, and P. Jena, Eds., Nova Science Publishers (2006).

[3] J. Bernholc, W. Lu, S. M. Nakhmanson, V. Meunier, and M. Buongiorno Nardelli, *Multiscale simulations of quantum structures,* Proceedings of DoD 2005 Users Group Conference, IEEE Computer Society, pp. 18–24 (2005).

[2] J. Bernholc, M. Buongiorno Nardelli, W. Lu, V. Meunier, S. M. Nakhmanson, and Q. Zhao, *Large-scale quantum-mechanical simulations of nanoscale devices and new materials,* Proceedings of DoD 2004 Users Group Conference, IEEE Computer Society, pp. 34–38 (2004).

[1] J. Bernholc, M. Buongiorno Nardelli, W. Lu, V. Meunier, S. Nakhmanson and Q. Zhao, *Simulations of nanotube-based structures and devices,* Proc. Conf. on Foundations of Nanoscience: Self-assembled Architectures and Devices, Science Technica, p. 367 (2004).

Presentations

Invited talks and tutorials at major conferences/symposia

25. *Ferret: an open-source code for simulating thermodynamical evolution and phase transformations in complex materials systems at mesoscale*, MS&T Meeting, Pittsburgh PA, Oct 2017.

24. *Ferret: an open-source code for simulating thermodynamical evolution and phase transformations in complex materials systems at mesoscale*, MRS Spring Meeting, Phoenix AZ, Apr 2017.

23. *Fun with functional oxide layers: from atomic scale to mesoscale*, 5th International Conference from Nanoparticles and Nanomaterials to Nanodevices and Nanosystems (IC4N), Porto Heli, Greece, June 26–30, 2016.
22. *Unusual ferroic functionalities in complex-oxide multilayers by design: from atomic scale to mesoscale*, XXIV International Materials Research Congress (IMRC), Cancun, Mexico, August 16–20, 2015.
21. *Complex-oxide multilayers by design: a treasure trove of unusual ferroic functionalities*, APS March Meeting, San Antonio TX, March 2–6, 2015.
20. *Complex-oxide multilayers by design: a treasure trove of unusual ferroic functionalities*, ACerS Electronic Materials and Applications Meeting, Orlando FL, January 21–23, 2015.
19. *Multiscale modeling of layered electroactive materials*, 8th Energy Materials Nanotechnology (EMN) Fall Meeting, Orlando FL, November 22–25, 2014.
18. *Computational design of multifunctional layered-oxide materials across length scales*, XXI Czech-Polish seminar on structural and ferroelectric phase transitions, Sezimovo Usti, Czech Republic, May 19–23, 2014.
17. *Computational design of multifunctional layered oxides across length scales*, ACerS Electronic Materials and Applications Meeting, Orlando FL, January 22–24, 2014.
16. *Elastic Properties of Coupled Mesoscale Systems,* (given by S. Gu, with B. Lee, S. Hong, O. Heinonen, D. Karpeev) 12th U.S. National Congress on Computational Mechanics, Raleigh NC, July 22–25, 2013.
15. *Ab initio design of layered ferroic materials for advanced functionalities*, 4th International Conference from Nanoparticles and Nanomaterials to Nanodevices and Nanosystems (IC4N), Corfu, Greece, June 2013.
14. *Materials Genome Initiatives at the University of Connecticut*, (given by S. P. Alpay) MRS Spring Meeting, San Francisco CA, Apr 1–5, 2013.
13. *Ab initio design of morphotropic phase boundaries in ferroic materials for advanced functionalities*, MRS Spring Meeting, San Francisco CA, Apr 1–5, 2013.
12. *Ab initio design of ferroic materials with advanced functionalities: 2D ferroelectricity and Goldstone-like modes in perovskite-oxide layers*, ACerS Electronic Materials and Applications Meeting, Orlando FL, Jan 23–25, 2013.
11. *Ab initio design of ferroic materials with advanced functionalities: 2D ferroelectricity and Goldstone-like modes in perovskite-oxide layers*, International Symposium on Integrated Functionalities, Hong Kong, PRC, Jun 18–21, 2012.
10. *Electroactive nanotube and polymer compounds by first principles design*, International Workshop on Composites of Inorganic Nanotubes and Polymers, Institute of Physics ASCR, Prague, Czech Republic, Apr 17–20, 2012.
9. *Perovskite Ferroelectric $SnTiO_3$: Myth or Reality? A First-Principles Investigation,* (with W. D. Parker and J. M. Rondinelli), International Symposium on Integrated Functionalities, Cambridge UK, Aug 1–4, 2011.

8. *Electroactive properties of ferroelectric polyvinylidene fluoride and related copolymer and oligomer compounds* (with M. Buongiorno Nardelli, J. Bernholc, R. Korlacki, J. M. Takacs, and S. Ducharme), International School and Symposium on Multifunctional Molecule-based Materials, Argonne National Lab, Argonne IL, March 13–18, 2011.
7. *First principles calculations of polarization and phonons in ferroelectric materials with Quantum Espresso,* tutorial for the International Symposium on Integrated Functionalities, San Juan PR, June 13–16, 2010.
6. *Putting the groove back into ferroelectric oxides: a prediction of Goldstone-like states in a layered perovskite with frustrated polarization* (with I. Naumov), TW physical society meeting, Tainan, Taiwan, Feb 1–5, 2010.
5. *Putting the groove back into ferroelectric oxides: a prediction of Goldstone-like states in a layered perovskite with frustrated polarization* (with I. Naumov), TW-ANL workshop, Tainan, Taiwan, Feb 1–5, 2010.
4. *Polarization and dynamics in ferroelectric β-polyvinylidene fluoride and related copolymer and oligomer compounds* (with R. Korlacki, J. Travis Johnson, S. Ducharme, Z. Ge, J. M. Takacs, J. Bernholc, and M. Buongiorno Nardelli), International Symposium on Integrated Ferroelectrics and Functionalities, Colorado Springs CO, September 2009.
3. *Understanding, enhancing and fine-tuning polar properties in multicomponent perovskite superlattices* (with K. M. Rabe and D. Vanderbilt), APS March Meeting, Denver CO, March 2007.
2. *Design of new ferroelectric polymers through computer simulations* (with J. Bernholc, and M. Buongiorno Nardelli), 16-th Annual Workshop on Recent Developments in Electronic Structure Methods, New Brunswick NJ, May 2004.
1. *Designing novel polar materials through computer simulations* (with J. Bernholc, and M. Buongiorno Nardelli), Mardi Gras Physics conference, Baton Rouge LA, February 2003.

Seminars and Colloquiua

33. *Ferret: an open-source code for simulating thermodynamical evolution and phase transformations in complex materials systems at mesoscale*, Department of Physics, University of Geneva, Switzerland, May 2017.
32. *Fun with functional oxides: from atomic scale to mesoscale,* Army Research Lab, Washington D.C., Dec 2016.
31. *Fun with functional oxide layers: from atomic scale to mesoscale*, Oak Ridge National Lab, Oak Ridge TN, July 2016.
30. *Fun with functional oxide layers: from atomic scale to mesoscale*, Department of Physics and Astronomy, SUNY Stony Brook, May 2016.
29. *Unusual ferroic functionalities in complex-oxide multilayers by design*, MSD Colloquium, Argonne National Lab, Argonne IL, July 23, 2015.

28. *Computational Design of Multifunctional Complex-oxide Materials Across Length Scales*, Ohio University Physics Department Colloquium, Athens OH, March 2014.
27. *Ab initio design of ferroic materials with advanced functionalities: 2D ferroelectricity and Goldstone-like modes in perovskite-oxide layers,* Department of Physics and Astronomy, University of Nebraska, Lincoln NE, June 4, 2012.
26. *Ab initio design of multifunctional materials with advanced properties: Goldstone-like states in a layered perovskite with constrained polarization,* Institute of Physics ASCR, Prague, Czech Republic, April 2012.
25. *Putting the groove back into ferroelectric oxides: Goldstone-like ferroelectricity by first principles design,* Yale University, New Haven CT, Oct 19, 2011.
24. *Putting the groove back into ferroelectric oxides: Goldstone-like ferroelectricity by first principles design,* Central Michigan University, Mt. Pleasant MI, Sep 1, 2011.
23. *Putting the groove back into ferroelectric oxides: Goldstone-like ferroelectricity by first principles design,* Imperial College London and the Thomas Young Centre for theory and simulation of materials, London UK, Aug 9, 2011.
22. *Putting the groove back into ferroelectric oxides: Goldstone-like ferroelectricity by first principles design,* National Physical Laboratory, Teddington UK Aug 8, 2011.
21. *Putting the groove back into ferroelectric oxides: a prediction of Goldstone-like states in a layered perovskite with constrained polarization,* University of South Florida, Tampa FL, September 17, 2010.
20. *Goldstone Ferroelectricity by First Principles Design,* ANL/Ames Lab M2D2 Strategic Initiative-Sponsored Workshop, Argonne IL, June 7–8, 2010.
19. *Putting the groove back into ferroelectric oxides: a prediction of Goldstone-like states in a layered perovskite with frustrated polarization,* Oak Ridge National Lab, Oak Ridge TN, May 25, 2010.
18. *Putting the groove back into ferroelectric oxides: a prediction of Goldstone-like states in a layered perovskite with frustrated polarization,* University of Illinois Chicago, Chicago IL, April 15, 2010.
17. *Understanding, enhancing and fine-tuning polar properties in novel ferroelectric materials*, University of Wisconsin-Madison, Madison WI, March 2009.
16. *Understanding, enhancing and fine-tuning polar properties in multicomponent perovskite materials*, MSD Colloquium, Argonne National Lab, Argonne IL, June 2007.
15. *First-principles studies of polarization control and enhancement in novel ferroelectric materials*, Auburn University, Auburn AL, October 2006.
14. *First-principles studies of polarization control and enhancement in novel ferroelectric materials*, Argonne National Lab, Argonne IL, March 2006.
13. *Ab initio studies and design of ferroelectric-polymer materials*, CMSS seminar, Department of Physics & Astronomy, Ohio University, Athens OH, October 2005.
12. *Ab initio studies and design of ferroelectric polymers*, Steklov Institute of Mathematics (St-Petersburg department), St-Petersburg, Russia, June 2005.

11. *Design of new ferroelectric polymers through computer simulations*, Department of Physics and Astronomy, Rutgers, Piscataway NJ, April 2004.
10. *Design of new ferroelectric polymers through computer simulations*, Department of Physics, Ohio State University, Columbus OH, April 2004.
9. *Design of new ferroelectric polymers through computer simulations*, Department of Physics and Astronomy, University of Nebraska, Lincoln NE, April 2004.
8. *New piezoelectric and pyroelectric materials by first principles design*, Center for Computational Materials Science, Naval Research Lab, Washington DC, October 2003.
7. *Designing new polar materials on a computer*, Steklov Institute of Mathematics (St-Petersburg department), St-Petersburg, Russia, June 2003.
6. *Designing new polar materials on a computer*, Department of Semiconductor Physics and Nanoelectronics, St-Petersburg State Technical University, St-Petersburg, Russia, June 2003.
5. *Designing new polar materials on a computer*, CMSS seminar, Department of Physics & Astronomy, Ohio University, Athens OH, March 2003.
4. *Spontaneous polarization and piezoelectricity in boron-nitride nanotubes*, Condensed Matter Seminar, Department of Physics, Universite de Montreal, Montreal (Quebec), Canada, October 2002.
3. *Realistic Models of Paracrystalline Silicon*, Department of Materials Science & Engineering, UIUC, Urbana IL, November 2001.
2. *Realistic Models of Paracrystalline Silicon*, CMSS Seminar, Department of Physics & Astronomy, Ohio University, Athens OH, February 2001.
1. *Paired states in homogeneous low-density electron gas*, Steklov Institute of Mathematics (St-Petersburg department), St-Petersburg, Russia, 1996.

Contributed talks

70. *A First-Principles Based Design of Organic Ferroelectrics: The Case of PVDF and DIPA Materials Templates,* (A. Ghosh, L. Louis, A. Asandei), NSF/CECAM School on Computational Materials Science: From Basics to Applications, CECAM, EPFL, Lausanne, Switzerland, July 17–27, 2017.
69. *Ferroelectric domain alignment in $PbTiO_3/SrTiO_3$ superlattice nanostructures,* (J. Park, J. Mangeri, P. Evans), APS March Meeting, New Orleans LA, March 2017.
68. *First-principles-based Landau energy functionals for perovskite ferroelectrics,* (K. C. Pitike, J. Mangeri, V. Cooper), APS March Meeting, New Orleans LA, March 2017.
67. *Intrinsic size effects and topological phase transformations in ferroelectric nanoparticles embedded in dielectric media,* (J. Mangeri, Y. Espinal, P. Alpay, O. Heinonen), APS March Meeting, New Orleans LA, March 2017.

66. *Ferret: an open-source code for simulating thermodynamical evolution and phase transformations in complex materials systems at mesoscale,* (K. C. Pitike, J. Mangeri, L. Kuna, P. Alpay, O. Heinonen), APS March Meeting, New Orleans LA, March 2017.

65. *Room Temperature Ferroelectricity and Photovoltaic Effect in Atomic Layer Deposited $SnTiO_x$ Thin Films,* (R. Agarwal, C. Takoudis, S. Hong), APS March Meeting, New Orleans LA, March 2017.

64. *Chemistry, Growth Kinetics and Epitaxial Stabilization of Sn^{2+} in Sn-Doped $SrTiO_3$ Using $(CH_3)_6Sn_2$ Tin Precursor,* (T. Wang, K. C. Pitike, B. Jalan), ACerS Electronic Materials and Applications Meeting, Orlando FL, Jan 2017.

63. *Intrinsic size effects and topological phase transformations in ferroelectric nanoinclusions embedded in a dielectric matrix,* (J. Mangeri, Y. Espinal, P. Alpay, O. Heinonen), ACerS Electronic Materials and Applications Meeting, Orlando FL, Jan 2017.

62. *Ferret: An open-source code for simulating materials thermodynamics at mesoscale,* (K. C. Pitike, J. Mangeri, L. Kuna, P. Alpay, O. Heinonen), ACerS Electronic Materials and Applications Meeting, Orlando FL, Jan 2017.

61. *First-principles-based Landau energy functionals for perovskite ferroelectrics,* (K. C. Pitike, J. Mangeri, V. Cooper), ACerS Electronic Materials and Applications Meeting, Orlando FL, Jan 2017.

60. *Temperature-induced ferroelectric phase transition in ABO_3 perovskites: A Wang-Landau-DFT approach,* (S. Yuk, K. C. Pitike, V. Cooper), ACerS Electronic Materials and Applications Meeting, Orlando FL, Jan 2017.

59. *Mesoscale Simulations of the Influence of Elastic Strains on the Optical Properties of Semiconducting Core-Shell Nanowires,* (L. Kuna, J. Mangeri, P.-X. Gao), MRS Fall meeting, Nov 2016.

58. *Ab Initio Studies of Polar Properties of Tetrafluoropropene/Vinylidene Fluoride Copolymers,* (A. Ghosh, L. Louis, A. Asandei), MRS Fall meeting, Nov 2016.

57. *First principles studies of diisopropylammonium-based molecular-ferroelectric crystals,* (L. Louis, S. Poddar, S. Ducharme), MRS Fall meeting, Nov 2016.

56. *Quantum Mechanical pKa Prediction of Drug-Like Molecules,* (L. Louis, R. Stern, G. Wood), MRS Fall meeting, Nov 2016.

55. *Predicting Crystallization Propensity Using Machine Learning Approaches,* (A. Ghosh + Pfizer collaborators), MRS Fall meeting, Nov 2016.

54. *Chemistry, Growth Kinetics and Epitaxial Stabilization of Sn^{2+} in Sn-Doped $SrTiO_3$ Using $(CH_3)_6Sn_2$ Tin Precursor,* (T. Wang, K. C. Pitike, B. Jalan), MRS Fall meeting, Nov 2016.

53. *First-principles-based Landau Energy Functionals for Perovskite Ferroelectrics from a Machine Learning Approach,* (K. C. Pitike), MRS Fall meeting, Nov 2016.

52. *The origins of Goldstone-like polar distortions in perovskite-oxide multilayers*, (with K. C. Pitike and L. Louis), ACerS Electronic Materials and Applications Meeting, Orlando FL, Jan 20–22, 2016.

51. *Electrocaloric effects in layered oxides with easy polarization rotation*, (with J. Mangeri, K. C. Pitike and S. P. Alpay), ACerS Electronic Materials and Applications Meeting, Orlando FL, Jan 20–22, 2016.

50. *Unusual ferroic functionalities in complex-oxide multilayers by design*, European Meeting on Ferroelectricity, Porto, Portugal, June 28 – July 3, 2015.

49. *Mesoscale modeling of functional properties in core-shell nanoparticles* (with J. Mangeri, O. Heinonen and D. Karpeev), APS March Meeting, San Antonio TX, March 2–6, 2015.

48. *First-principles studies of lone-pair-induced distortions in epitaxial phases of perovskite $SnTiO_3$ and $PbTiO_3$* (with K. C. Pitike, W. D. Parker and L. Louis), APS March Meeting, San Antonio TX, March 2–6, 2015.

47. *Structural and dielectric properties of the Ruddlesden-Popper Ba_2ZrO_4 structure from first-principles* (with L. Louis), Workshop on Fundamental Physics of Ferroelectrics and Related Materials, Oak Ridge National Lab, Oak Ridge TN, Jan 25–28, 2015.

46. *Mesoscale modeling of functional properties in core-shell nanoparticles* (with J. Mangeri, O. Heinonen and D. Karpeev), ACerS Electronic Materials and Applications Meeting, Orlando FL, January 21–23, 2015.

45. *Polarization "doughnut" states in layered-oxide nanostructures*, XXII International Materials Research Congress (IMRC), Cancun, Mexico, August 2013.

44. *Epitaxial strain tuning of polarization and band gap in perovksite $SnTiO_3$* (with W. Parker and J. Rondinelli), APS March meeting, Boston MA, Feb 27 – Mar 2, 2012.

43. *Epitaxial Strain Tunes Polarization and Electronic Band Gap in perovskite $SnTiO_3$* (with W. Parker and J. Rondinelli), Workshop on Fundamental Physics of Ferroelectrics and Related Materials, Argonne National Lab, Argonne IL, Jan 29 – Feb 1, 2012.

42. *Probing Ferroelectricity in Thin-film Perovskite $SnTiO_3$ with First-principles Structural Instability Analysis* (with W. Parker and J. Rondinelli), APS March meeting, Dallas TX, Mar 21–25, 2011.

41. *Anatomy of the Goldstone-like effect in a phason-ferroelectric layered perovskite oxide* (with I. Naumov), Workshop on Fundamental Physics of Ferroelectrics and Related Materials, National Institute of Standards and Technology (NIST), Gaithersburg MD, Jan 30 – Feb 2, 2011.

40. *Infrared spectroscopy of the soft mode and acoustic phonons in epitaxial $BaTiO_3$/ $SrTiO_3$ superlattices* (with V. Železný, A. Soukiassian, X. X. Xi, D. G. Schlom, J. Hlinka, Ch. Kadlec), Workshop on Fundamental Physics of Ferroelectrics and Related Materials, National Institute of Standards and Technology (NIST), Gaithersburg MD, Jan 30 – Feb 2, 2011.

39. *Putting the groove back into ferroelectric oxides: a prediction of Goldstone-like states in a layered perovskite with frustrated polarization* (with I. Naumov), International Symposium on Integrated Functionalities, San Juan PR, June 13–16, 2010.

38. *Quantitative Probes for the Functional Properties of Ferroelectric/Dielectric Superlattices* (with J. Y. Jo, R. Sichel, P. Chen, R. Smith, H.-N. Lee, E. Dufresne, and P. G. Evans), International Symposium on Integrated Functionalities, San Juan PR, June 13–16, 2010.

37. *Goldstone-like states in a layered perovskite with frustrated polarization* (with I. Naumov), APS March meeting, Portland OR, Mar 15–19, 2010.

36. *Piezoelectric response of epitaxial ferroelectric heterostructures* (with J. Y. Jo, R. Sichel, H.-N. Lee, E. Dufresne, and P. G. Evans), APS March meeting, Portland OR, Mar 15–19, 2010.

35. *First-principles studies of ultrathin ferroelectric capacitors with Ru-based perovskite electrodes* (with J. He and V. Cooper), APS March meeting, Portland OR, Mar 15–19, 2010.

34. *Vibrational Properties of Ferroelectric β-Vinylidene Fluoride Polymers and Oligomers* (with R. Korlacki, J. Travis Johnson, S. Ducharme, Z. Ge, J. M. Takacs), Fall MRS meeting, Boston MA, Nov 30 – Dec 4, 2009.

33. *Synchrotron X-ray Probe for Structural Evolution of Ferroelectric Heterostructure Thin Films* (with J. Y. Jo *et al*), Fall MRS meeting, Boston MA, Nov 30 – Dec 4, 2009.

32. *Understanding the Surface Reconstruction during Chemical Switching of Ultrathin $PbTiO_3$ Films from Density Functional Theory* (with J. He and B. Stephenson), Argonne Postdoctoral Research symposium, Argonne IL, September 2009.

31. *Phase transitions in vinylidene fluoride oligomers* (with R. Korlacki, J. Travis Johnson, S. Ducharme, Z. Ge, J. M. Takacs), International Symposium on Integrated Ferroelectrics and Functionalities, Colorado Springs CO, September 2009.

30. *Phase diagram in strained epitaxial $BaTiO_3/SrTiO_3$ superlattices studied by ultraviolet Raman spectroscopy* (with D. A. Tenne, A. Soukiassian, X. X. Xi, and D. G. Schlom), APS March Meeting, Pittsburgh PA, March 2009.

29. *Understanding the surface reconstruction during chemical switching of ultrathin $PbTiO_3$ films from density functional theory* (with J. He and B. Stephenson), APS March Meeting, Pittsburgh PA, March 2009.

28. *Polarization rotation in epitaxially strained perovskite-oxide superlattices*, APS March Meeting, Pittsburgh PA, March 2009.

27. *Phase diagram in strained $BaTiO_3/SrTiO_3$ superlattices: a UV Raman study* (with D. A. Tenne, A. Soukiassian, X. X. Xi, and D. G. Schlom), Workshop on Fundamental Physics of Ferroelectrics, Williamsburg VA, February 2009.

26. *Vibrational properties of ferroelectric β-polyvinylidene fluoride* (with R. Korlacki and S. Ducharme), Workshop on Fundamental Physics of Ferroelectrics, Williamsburg VA, February 2009.

25. *Tuning the structural instabilities in layered-perovskite ferroelectrics by epitaxial strain*, Workshop on Fundamental Physics of Ferroelectrics, Williamsburg VA, February 2009.

24. *The effects of surface and interface compensation on the polarization in ferroelectric $PbTiO_3$ ultrathin films* (with J. He and B. Stephenson), Argonne Postdoctoral Research symposium, Argonne IL, September 2008.

23. *The effects of surface and interface compensation on the polarization in ferroelectric $PbTiO_3$ ultrathin films* (with J. He and B. Stephenson), Workshop on Recent Developments in Electronic Structure Methods, Champaign IL, June 2008.

22. *Competing structural instabilities in Ti-based layered-perovskite-oxide superlattices* APS March Meeting, New Orleans LA, March 2008.

21. *Critical thickness for ferroelectricity in ultrathin perovskite films with inequivalent electrodes* Workshop on Fundamental Physics of Ferroelectrics, Williamsburg VA, February 2008.

20. *Strain-polarization coupling in epitaxial perovskites: A comparison between A-site and B-site driven ferroelectrics* (with H. N. Lee), Workshop on Fundamental Physics of Ferroelectrics, Williamsburg VA, February 2007.

19. *Predicting polarization enhancement in multicomponent ferroelectric superlattices* (with K. M. Rabe and D. Vanderbilt), APS March Meeting, Baltimore MD, March 2006.

18. *Weak strain-polarization coupling and ferroelectricity in epitaxially strained PZT (ultra)thin films* (with H. N. Lee), Workshop on Fundamental Physics of Ferroelectrics, Williamsburg VA, February 2006.

17. *Revealing the hidden polar character of $CaTiO_3$* (with A. Zayak and K. M. Rabe), Workshop on Fundamental Physics of Ferroelectrics, Williamsburg VA, February 2006.

16. *Predicting polarization enhancement in multicomponent ferroelectric superlattices* (with K. M. Rabe and D. Vanderbilt), Workshop on Fundamental Physics of Ferroelectrics, Williamsburg VA, February 2006.

15. *Polarization enhancement in two- and three-component ferroelectric superlattices* (with K. M. Rabe and D. Vanderbilt), ACS Meeting, Washington DC, August 2005.

14. *Polarization enhancement in two- and three-component ferroelectric superlattices* (with K. M. Rabe and D. Vanderbilt), Workshop on Recent Developments in Electronic Structure Methods, Ithaca NY, June 2005.

13. *First principles studies of self-polarization in electroactive polymers* (with M. Buongiorno Nardelli and J. Bernholc), APS March Meeting, Los Angeles CA, March 2005.

12. *Polarization enhancement in two- and three-component ferroelectric superlattices* (with K. M. Rabe and D. Vanderbilt), Workshop on Fundamental Physics of Ferroelectrics, Williamsburg VA, February 2005.

11. *Superpolar polymers by first principles design* (with M. Buongiorno Nardelli and J. Bernholc), APS March Meeting, Montreal (Quebec), Canada, March 2004.
10. *Superpolar polymers by design* (with M. Buongiorno Nardelli and J. Bernholc), Workshop on Fundamental Physics of Ferroelectrics, Williamsburg VA, February 2004.
9. *Polar properties of ferroelectric polymers from the first principles* (with M. Buongiorno Nardelli and J. Bernholc), APS March Meeting, Austin TX, March 2003.
8. *Spontaneous polarization and piezoelectric properties of boron-nitride nanotubes* (with M. Buongiorno Nardelli and J. Bernholc), Nanotube 2002, Boston College, Boston MA, July 2002.
7. *Spontaneous polarization and piezoelectric response in BN nanotubes* (with M. Buongiorno Nardelli and J. Bernholc), APS March Meeting, Indianapolis IN, March 2002.
6. *Realistic Models of Paracrystalline Silicon* (with D. A. Drabold, N. Mousseau and P. M. Voyles), APS March Meeting, Seattle WA, March 2001.
5. *Models of Paracrystalline Silicon with a Defect-Free Bandgap* (with D. A. Drabold), Midwest Solid State Conference and Solid State Theory Symposium, University of North Dakota, Grand Forks ND, October 2000.
4. *Computer simulation for the low-temperature anomalous specific heat in amorphous silicon with voids* (with D. A. Drabold), APS March Meeting, Minneapolis MN, March 2000.
3. *Computer simulation of low-energy excitations and specific heat in a-Si* (with D. A. Drabold), Midwest Solid State Conference, Ohio University, Athens OH, October 1999.
2. *Computer simulation of low-energy excitations in amorphous silicon* (with D. A. Drabold), ICAMS18, Snowbird UT, August 1999.
1. *Vibrational signatures of void-type defects in amorphous silicon* (with D. A. Drabold), APS March Meeting, Atlanta GA, March 1999.