

RESUME OF INNA PONOMAREVA

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• Career/Employment

2013/present	Associate Professor	University of South Florida.
2009/2013	Assistant Professor	University of South Florida.
2007/2009	Research Associate Professor	University of Arkansas.
2006/2007	Research Assistant Professor	University of Arkansas.
2004/2006	Research Associate	University of Arkansas.

• Education

2004	Ph.D. in Physics	Institute of Biochemical Physics of Russian Academy of Sciences.
2001	Master of Physics	Volgograd State University, Russia.
1996	High-school graduate	Volgograd, high-school N 130, Russia.

• Grants Awarded

Single PI grants

- 09/01/2013-08/31/2018: *"CAREER: Towards universal understanding of caloric and other complex effects in ferroics from multiscale modeling"*, National Science Foundation, DMR-1250492 (\$435,000).
- 09/01/2013-08/31/2016: *"Complex (anti)ferroic oxides: statics and dynamics at finite temperatures"*, U.S. Department of Energy, Office of Basic Energy Sciences, Grant DE-SC0005245 (\$405,000).
- 09/01/2011-08/31/2014: *"Terahertz Nanoscience of Multifunctional materials: Atomistic Exploration"*, Army Research Office, Department of Defense, Contract 57787-EL (\$412,756).
- 09/01/2010-08/31/2013: *"Atomistic Study of Ultrafast Dynamics in Multifunctional Materials in Bulk and Nanoforms"*, U.S. Department of Energy, Office of Basic Energy Sciences, Grant DE-SC0005245 (\$405,000).

- **Publications and Citation Metrics**

As of 09/11/2013 from Web of Knowledge database

Total number of peer-reviewed publications: 50

Total citation index: 1027

Average citation per article: 21

h-index: 18

- **Teaching and Outreach**

Graduate level courses: Computational Nanoscience (2008), Computational Physics I (2009-2013). Students evaluation score from the last semester is 4.9/5.0.

Undergraduate level courses: Mathematical Methods in Physics (2009-2013). Students evaluation score from the last semester is 4.3/5.0.

PostDocs, graduate, undergraduate students, and other advising: Three PostDocs, four graduate students, four undergraduate students, and one high-school student. One PhD and one Master degree in Applied Physics awarded to the advisees.

Outreach: Developer and coordinator for an outreach program targeting middle school students (<http://shell.cas.usf.edu/~iponomar/outreach.html>). The program is recognized by NSF CAREER award.

- **Research Synopsis and Professional Expertise**

Research Fields: Computational condensed matter physics and nanoscience, numerical quantum chemistry, computational techniques development and implementation;

Areas of expertise: semiconductors, complex ferroics, multiferroics and antiferroics, low-dimensional structures;

Research interests: static and dynamic properties of ferroics at finite temperatures and at the nanoscale, phase transitions, mechanics at the nanoscale, flexoelectricity, caloric effects, predictive modeling, high-performance computing;

Computational techniques: *Ab initio* density-functional-theory based methods, Classical and Quantum-mechanical Molecular Dynamics, classical Monte Carlo, empirical potentials, tight-binding electronic structure methods and Molecular Dynamics, effective Hamiltonian techniques.

Professional expertise: Reviewer for Physical Review Letters, Physical Review B, Computational Materials Science, Journal of Applied Physics, Physica E, Applied Physics Letters, European Physical Journal Plus, and Physica Status Solidi. Reviewer for National Science Foundation, U.S. Department of State, U.S. Department of Energy.

- **U.S. patents**

“Asymmetric dipolar rings”, Patent number 7,835,168.

- **Most significant works**

1. B. K. Mani, C.-M. Chang, and I. Ponomareva, “Atomistic study of soft-mode dynamics in PbTiO_3 ”, Phys. Rev. B **88**, 064306 (2013).

2. S. Lisenkov, B. K. Mani, C.-M. Chang, J. Almand, and I. Ponomareva , “Multicaloric effect in ferroelectric PbTiO_3 from first principles ”, Phys. Rev. B **87**, 224101 (2013).
3. I. Ponomareva and S. Lisenkov, “Bridging the Macroscopic and Atomistic Descriptions of the Electrocaloric Effect”, Phys. Rev. Lett. **108**, 167604 (2012).
4. Kevin McCash, A. Srikanth, and I. Ponomareva, “Competing polarization reversal mechanisms in ferroelectric nanowires”, Phys. Rev. B **86**, 214108 (2012).
5. I. Ponomareva and S. Lisenkov, “Giant elastocaloric effect in ferroelectric $\text{Ba}_{0.5}\text{Sr}_{0.5}\text{TiO}_3$ alloys from first-principles”, Phys. Rev. B **86**, 104103 (2012).
6. I. Ponomareva, A. Tagantsev, and L. Bellaiche, “Finite-temperature flexoelectricity in ferroelectric thin films from first principles”, Phys. Rev. B. **85**, 104101 (2012).
7. Qingteng Zhang, R. Herchig and I. Ponomareva, “Nanodynamics of Ferroelectric Ultrathin Films”, Phys. Rev. Lett. **107**, 177601 (2011).
8. Qingteng Zhang and I. Ponomareva “Microscopic insight into temperature-graded ferroelectrics”, Phys. Rev. Lett. **105**, 147602 (2010).
9. S. Lisenkov and I. Ponomareva, “Intrinsic electrocaloric effect in ferroelectric alloys from atomistic simulations”, Phys. Rev. B., Rapid Com. **80**, 140102(R) (2009).
10. H. Bea, B. Dupe, S. Fusil, R. Mattana, E. Jacquet, B. Warot-Fonrose, F. Wilhelm, A. Rogalev, S. Petit, V. Cros, A. Anane, F. Petroff, K. Bouzehouane, G. Geneste, B. Dkhil, S. Lisenkov, I. Ponomareva, L. Bellaiche, M. Bibes, and A. Barthelémy, “A room-temperature multiferroic with a giant axial ratio”, Phys. Rev. Lett. **102**, 217603, (2009).
11. I. Ponomareva and L. Bellaiche, “Nature of dynamical coupling between polarization and strain in nanoscale ferroelectrics from first principles ”, Phys. Rev. Lett. **101**, 197602 (2008).
12. J. Hlinka, T. Ostapchuk, D. Nuzhnyy, J. Petzelt, P. Kuzel, C. Kadlec, P. Vanek, I. Ponomareva, L. Bellaiche, “Coexistence of the relaxation and soft modes in the terahertz dielectric response of tetragonal BaTiO_3 ”, Phys. Rev. Lett. **101**, 167402 (2008).
13. S. Prosandeev, I. Ponomareva, I. Kornev, and L. Bellaiche, “ Control of Vortices by Homogeneous Fields in Asymmetric Ferroelectric and Ferromagnetic Rings”, Phys. Rev. Lett. **100**, 047201 (2008).
14. I. Ponomareva, L. Bellaiche, T. Ostapchuk, J. Hlinka and J. Petzelt, “Terahertz dielectric response of cubic BaTiO_3 ”, Phys. Rev. B **77**, 012102 (2008).
15. I. Ponomareva, L. Bellaiche, and R. Resta, “Dielectric anomalies in ferroelectric nanostructures”, Phys. Rev. Lett. **99**, 227601 (2007).
16. Inna Ponomareva, Deepak Srivastava, and Madhu Menon, “Thermal Conductivity in Thin Silicon Nanowires: Phonon Confinement Effect”, Nano Lett., **7(5)**, 1155 (2007).

17. S. Prossandeev, I. Ponomareva, I. Kornev, I. Naumov and L. Bellaiche, “Controlling toroidal moment by means of an inhomogeneous static field: An *ab initio* study”, Phys. Rev. Lett. **96**, 237601 (2006).
18. B.-K. Lai, I. Ponomareva, I. I. Naumov, I. Kornev, H. Fu, L. Bellaiche, and G. J. Salamo, “Electric-Field-Induced Domain Evolution in Ferroelectric Ultrathin Films”, Phys. Rev. Lett. **96**, 137602 (2006).
19. I. Ponomareva, I. I. Naumov, I. Kornev, Huaxiang Fu and L. Bellaiche, “Atomistic treatment of depolarizing energy and field in ferroelectric nanostructures”, Phys. Rev. B, Rapid Com. **72**, 140102 (2005).
20. I. Ponomareva, M. Menon, D. Srivastava, and A.N. Andriotis, “Structure, Stability, and Quantum Conductivity of Small Diameter Silicon Nanowires”, Phys. Rev. Lett. **95**, 265502 (2005).
21. M. Menon, A. N. Andriotis, D. Srivastava, I. Ponomareva and L. A. Chernozatonskii, “Carbon Nanotube “T-junctions”: Formation Pathways and Conductivity”, Phys. Rev. Lett., **91**, 145501 (2003).

• Other Publications

22. Qingteng Zhang and I Ponomareva, “Depolarizing field in temperature-graded ferroelectrics from an atomistic viewpoint”, New J. Phys. **15**, 043022 (2013).
23. J. Weerasinghe, L. Bellaiche, T.Ostapchuk, P. Kuzel, C. Kadlec, S. Lisenkov, I. Ponomareva, J. Hlinka, “Emergence of central mode in the paraelectric phase of ferroelectric perovskites”, MRS Communications **3**, 42 (2013).
24. R Herchig, Kimberly Schultz, Kevin McCash and I Ponomareva, “Terahertz sensing using ferroelectric nanowires ”, Nanotechnology **24**, 045501 (2013).
25. S.Lisenkov, I. Ponomareva, and L. Bellaiche, “Central Mode in Disordered $(\text{Ba}_{0.6}\text{Sr}_{0.4})\text{TiO}_3$ Solid Solution from First Principles”, Proceedings of the High Performance Computing Modernization Program (2011).
26. L. Louis, P. Gemeiner, I. Ponomareva, L. Bellaiche, G. Geneste, W. Ma, N. Setter and B. Dkhil, “Low-Symmetry Phases in Ferroelectric Nanowires”, NanoLetters **10(4)**, 1177 (2010).
27. S. Bin-Omran, I. Kornev, I. Ponomareva, and L. Bellaiche, “Diffuse phase transitions in ferroelectric ultrathin films from first principles”, Phys. Rev. B **81**, 094119 (2010).
28. R. Michael Sheetz, Inna Ponomareva, Ernst Richter, Antonis N. Andriotis, and Madhu Menon, “Defect-induced optical absorption in the visible range in ZnO nanowires”, Phys. Rev. B **80**, 195314 (2009).
29. T. Ostapchuk, J Petzelt, J Hlinka, V Bovtun, P Kuzel, I Ponomareva, S Lisenkov, L Bellaiche, A. Tkach and P. Vilarinho, “Broad-band dielectric spectroscopy and ferroelectric soft-mode response in the $\text{Ba}_{0.6}\text{Sr}_{0.4}\text{TiO}_3$ solid solution”, J. Phys.: Cond. Matt. **21**, 474215 (2009).

30. David Sichuga, I. Ponomareva and L. Bellaiche, “Phase diagrams of epitaxial $\text{Pb}(\text{Zr,Ti})\text{O}_3$ ultrathin films from first principles”, Phys. Rev. B **80**, 134116 (2009).
31. S. Lisenkov, I. Ponomareva, and L. Bellaiche, “Unusual static and dynamical characteristics of domain evolution in ferroelectric superlattices”, Phys. Rev. B **79**, 024101 (2009).
32. S. Prosandeev, I. Ponomareva, and L. Bellaiche, “Electrocaloric effect in bulk and low-dimensional ferroelectrics from first principles”, Phys. Rev. B **78**, 052103 (2008).
33. Igor A. Kornev, B.-K. Lai, I. Naumov, I. Ponomareva, H. Fu, and Laurent Bellaiche, “Domains in Ferroelectric Nanostructures from First Principles”, in “Handbook of advanced dielectric piezoelectric and ferroelectric materials: Synthesis, properties and applications”, edited by Zuo-Guang Ye, Chapter 5, Woodhead Publishing Limited (2008).
34. S. Bin-Omran, I. Ponomareva and L. Bellaiche, “Dependence of polarization on epitaxial strain in ferroelectric ultrathin films from first principles”, Phys. Rev. B **77**, 144105 (2008).
35. S Prosandeev, I Ponomareva, I Naumov, I Kornev and L Bellaiche, “Original properties of dipole vortices in zero-dimensional ferroelectrics”, J. Phys.: Cond. Matt. **20**, 193201 (2008).
36. I. Ponomareva, L. Bellaiche, and R. Resta, “Relation between dielectric responses and polarization’s fluctuations in ferroelectric nanostructures”, Phys. Rev. B **76**, 235403 (2007).
37. I. Ponomareva, E. Richter, A.N. Andriotis, and M. Menon, “Oscillatory Band Gap behavior in Small Diameter Si-Clathrate”, Nano Lett. **7**(11), 3424 (2007).
38. Bo-Kuai Lai, I. Ponomareva, I. Kornev, L. Bellaiche, and G. Salamo, “Thickness dependency of 180° stripe domains in ferroelectric ultrathin films: a first-principles-based study”, Appl. Phys. Lett. **91**, 152909 (2007).
39. Bo-Kuai Lai, Inna Ponomareva, Igor A. Kornev, L. Bellaiche, and G. J. Salamo, “Domain evolution of BaTiO_3 ultrathin films under an electric field: A first-principles study”, Phys. Rev. B **75**, 085412 (2007).
40. I. Ponomareva, M. Menon, E. Richter and A.N. Andriotis, “Structural stability, electronic properties, and quantum conductivity of small-diameter silicon nanowires”, Phys. Rev. B **74**, 125311 (2006).
41. I. Ponomareva and L. Bellaiche, “Influence of growth orientation on the properties of ferroelectric ultra-thin films”, Phys. Rev. B **74**, 064102 (2006).
42. I. Ponomareva, I. I. Naumov and L. Bellaiche, “Low-dimensional ferroelectrics under different electrical and mechanical boundary conditions: Atomistic simulations”, Phys. Rev. B **72**, 214118 (2005).
43. I. Ponomareva, I.I. Naumov, I. Kornev, Huaxiang Fu and L. Bellaiche, “Modelling of nanoscale ferroelectrics from atomistic simulations”, *Current Opinion in Solid State and Materials Science* **9**, 114 (2005).

44. S. Lisenkov, A. N. Andriotis, I. Ponomareva, and M. Menon “Transport properties of carbon nanotubes with odd-numbered carbon rings”, Phys. Rev. B **72**, 113401 (2005)
45. S. Lisenkov, I. Ponomareva, L.A. Chernozatonskii, “Basic configuration of carbon nanotube Y-junctions: Structure and classification”, Physics of the Solid State **46**, 1529 (2004).
46. I. Ponomareva, L. Chernozatonskii, “Defect formation in carbon onion under Ar irradiation ”, JETP Lett. **79**, 375 (2004).
47. M. Menon, D. Srivastava, I. Ponomareva, L. Chernozatonskii, “Nanomechanics of Silicon Nanowires”, Phys. Rev. B **70**, 125313 (2004) .
48. L.A. Chernozatonskii, I.V. Ponomareva, “Carbon nanotube multiterminal junctions: structures, properties, synthesis and applications”, NATO-ASI2003, Kluwer Publishers, (2004).
49. L.A. Chernozatonskii, I.V. Ponomareva ”Formation of single carbon nanotube T-junctions”, Fullerenes, nanotubes and carbon nanostructures, **12**, 87 (2004).
50. L. Chernozatonskii, I. Ponomareva, “Sticking of carbon nanotube Y-junction branches”, JETP Lett. , **78**, 327 (2003).
51. I.V. Ponomareva, L.A. Chernozatonskii, A.N. Andriotis, M. Menon, “Formation pathways for single-wall carbon nanotube multiterminal junctions”, New J. of Phys., **5**, 119.1. (2003).
52. I.V. Ponomareva, L.A. Chernozatonskii, “How can carbon onion transform into diamond-like structure?”, Microelectronic Engineering, **69**, 625 (2003).
53. I. Ponomareva, L. Chernozatonskii, “Mechanism of carbon onion core transformation into diamond-like structure”, JETP Lett., **76**, 456 (2002).

• Recent Invited Presentations

1. I. Ponomareva, “Caloric effects in ferroelectric alloys from atomistic simulations” , Electronic Materials and Applications 2013, Orlando, USA 2013.
2. I. Ponomareva, “Atomistic Study of Ultrafast Dynamics in Multifunctional Materials in Bulk and Nanoforms”, Department of Energy Principle Investigator Meeting, Washington, D.C., USA 2012.
3. I. Ponomareva, “Atomistic simulations for materials research”, Northeastern University, Boston, USA, 2011.
4. I. Ponomareva, “Ferroelectric nanowires: Atomistic exploration”, Nanowires10, Heraklion, Greece, 2010.
5. Qingteng Zhang and I. Ponomareva, “Microscopic insight into temperature-graded ferroelectrics”, International Materials Research Congress, Cancun, Mexico, 2010.
6. L. Bellaiche, S. Lisenkov, I. Ponomareva and R. Resta, “Complex Phenomena in $\text{Ba}_{0.5}\text{Sr}_{0.5}\text{TiO}_3$ Alloys from Atomistic Simulations”, International Symposium on Integrated Ferroelectrics, Colorado Springs, USA 2009.

7. L. Bellaiche, S. Lisenkov, I. Ponomareva and R. Resta, “Atomistic Insight into Complex Phenomena in Ferroelectric Alloys”, International Materials Research Congress, Cancun, Mexico, 2009.
8. I. Ponomareva, “Properties of ferroelectric nanostructures”, American Physical Society Meeting, New Orleans, USA, 2008.