

Fei Xue

Department of Materials Science and Engineering
The Pennsylvania State University
N-355 Millennium Science Complex
University Park, PA 16802-5006

Office: (814) 865-0389
Mobile: (814) 954-2056
Email: xuefei5376@gmail.com

Education

- **Ph. D., Materials Science and Engineering (Minor: Computational Science)**
The Pennsylvania State University, Aug. 2010-Dec. 2015
- **B.S., Department of Physics & Kuang Yaming Honors School**
Nanjing University, Sept. 2006-June 2010

Research Experience

Feb. 2016-Present: Postdoctoral Researcher, Department of Materials Science and Engineering, The Pennsylvania State University. Advisor: Prof. Long-Qing Chen

Aug. 2010- Dec. 2015: Research Assistant, Department of Materials Science and Engineering, The Pennsylvania State University. Thesis Advisor: Prof. Long-Qing Chen

- DFT calculation and phase-field simulation on Ruddlesden-Popper ferroelectrics
- Phase-field simulation of ferroelectric domain structures in hexagonal manganites
- Landau theory and phase-field simulation on domain structures in BiFeO₃
- Structural and metal-insulating transition in correlated oxide VO₂
- Stress-induced low symmetry phases in KNbO₃
- Phase-field simulation of domain structures in PbZr_xTi_{1-x}O₃ bi-layers
- Monte Carlo simulation on the size effect in ferroelectric nanostructures

Publications

1. **F. Xue**, X. Wang, Y. Shi, S.-W. Cheong, and L.-Q. Chen, "Strain-induced incommensurate phases in hexagonal manganites", *Physical Review B* **96**, 104109 (2017)
2. D. Lee, J. Lee, K. Song, **F. Xue**, S.-Y. Choi, Y. Ma, J. Podkaminer, D. Liu, L.-Q. Chen, S. H. Oh, Z. Ma and C.-B. Eom, "Sharpened VO₂ phase transition via controlled release of epitaxial strain", *Nano Letters* **17**, 5614 (2017)

3. L. Xie, L. Li, C. A. Heikes, Y. Zhang, Z. Hong, P. Gao, C. T. Nelson, F. Xue, E. Kioupakis, L.-Q. Chen, D. G. Schlom, P. Wang, and X. Pan, "Giant Ferroelectric Polarization in Ultrathin Ferroelectrics via Boundary-Condition Engineering", *Advanced Materials*, 1701475 (2017)
4. Z. Liao, **F. Xue**, W. Sun, D. Song, Q. Zhang, J.-F. Li, L.-Q. Chen, and J. Zhu, "Reversible phase transition induced large piezoelectric response in Sm-doped BiFeO₃ with a composition near the morphotropic phase boundary", *Physical Review B* **95**, 214101 (2017)
5. **F. Xue**, Y. Ji, and L.-Q. Chen, "Theory of Strain Phase Separation and Strain Spinodal: Applications to Ferroelastic and Ferroelectric Systems", *Acta Materialia* **133**, 147 (2017)
6. D. V. Karpinsky, E. A. Eliseev, **F. Xue**, M. V. Silibin, A. Franz, M. D. Glinchuk, I. O. Troyanchuk, S. A. Gavrilov, V. Gopalan, L.-Q. Chen, and A. N. Morozovska, "Thermodynamic Potential and Phase Diagram for Multiferroic Bismuth Ferrite (BiFeO₃)", *npj Computational Materials* **3**, 20 (2017)
7. Z. Hong, A. R. Damodaran, **F. Xue**, S.-L. Hsu, J. Britson, A. K. Yadav, C. T. Nelson, J.-J. Wang, J. F. Scott, L. W. Martin, R. Ramesh, and L.-Q. Chen, "Stability of Polar Vortex Lattice in Ferroelectric Superlattices", *Nano Letters* **17**, 2246 (2017)
8. **F. Xue**, Y. Li, Y. Gu, J. Zhang, and L.-Q. Chen, "Strain phase separation: Formation of ferroelastic domain structures", *Physical Review B* **94**, 220101(R) (2016)
9. Y. H. Hsieh, **F. Xue**, T. Yang, H. J. Liu, Y. Zhu, Y. C. Chen, Q. Zhan, C. G. Duan, L.-Q. Chen, Q. He, and Y. H. Chu, "Permanent ferroelectric retention of BiFeO₃ mesocrystal", *Nature Communications* **7**, 13199 (2016)
10. L. Li, **F. Xue**, C. Nelson, A. Melville, C. Heikes, D. Schlom, L.-Q. Chen, and X. Pan, "Size Effect on Spontaneous Flux-closure Domains in BiFeO₃ Thin Films", *Microscopy and Microanalysis* **22**, 1596 (2016)
11. **F. Xue**, L. Li, J. Britson, Z. Hong, C. A. Heikes, C. Adamo, D. G. Schlom, X. Pan, and L.-Q. Chen, "Switching the curl of polarization vectors by an irrotational electric field", *Physical Review B* **94**, 100103(R) (2016)
12. N. Quackenbush, H. Paik, M. Wahila, S. Sallis, M. Holtz, X. Huang, A. Ganose, B. Morgan, D. O. Scanlon, Y. Gu, **F. Xue**, L.-Q. Chen, G. E. Sterbinsky, C. Schlueter, T.-L. Lee, J. C. Woicik, J.-H. Guo, J. D. Brock, D. A. Muller, D. A. Arena, D. G. Schlom, and L. F. J. Piper, "Stability of the M2 phase of vanadium dioxide induced by coherent epitaxial strain", *Physical Review B* **94**, 085105 (2016)
13. F.-T. Huang, **F. Xue**, B. Gao, L. Wang, X. Luo, W. Cai, X.-Z. Lu, J. M. Rondinelli, L.-Q. Chen, and S.-W. Cheong, "Domain topology and domain switching kinetics in a hybrid improper ferroelectric", *Nature Communications* **7**, 11602 (2016)

14. H. Guo, X. Liu, **F. Xue**, L.-Q. Chen, W. Hong, and X. Tan, “Disrupting long-range polar order with an electric field”, *Physical Review B* **93**, 174114 (2016)
15. C. Ju, J. C. Yang, C. Luo, P. Shafer, H. J. Liu, Y. L. Huang, H. H. Kuo, **F. Xue**, C. W. Luo, L.-Q. Chen, Q. He, P. Yu, E. Arenholz, X. M. Lu, and Y. H. Chu, “Anomalous Electronic Anisotropy Triggered by Ferroelastic Coupling in Multiferroic Heterostructures”, *Advanced Materials* **28**, 876 (2016)
16. Q. Li, Y. Cao, P. Yu, R. Vasudevan, N. Laanait, A. Tselev, **F. Xue**, L.-Q. Chen, P. Maksymovych, S. Kalinin, and N. Balke, “Giant elastic tunability in strained BiFeO₃ near an electrically-induced phase transition”, *Nature Communications* **6**, 8985 (2015)
17. **F. Xue**, X. Wang, I. Socolenco, Y. Gu, L.-Q. Chen, and S.-W. Cheong, “Evolution of the statistical distribution in a topological defect network”, *Scientific Reports* **5**, 17057 (2015)
18. C. Ju, **F. Xue**, F. Huang, L.-Q. Chen, X. Lu, J. Zhu, H. M. Jensen, “Anomalous crack arrays in anisotropic-strained manganite on rare-earth scandate substrate”, *Applied Physics Letters* **106**, 201905 (2015)
19. Y. Gu, N. Wang, **F. Xue**, and L.-Q. Chen, “Origin of interfacial polar order in incipient ferroelectrics”, *Physical Review B* **91**, 174103 (2015)
20. Y. J. Li, J. J. Wang, J. C. Ye, X. Ke, G. Y. Gou, Y. Wei, **F. Xue**, J. Wang, C. S. Wang, R. C. Peng, X. Deng, Y. Yang, X. Ren, L.-Q. Chen, C.-W. Nan, and J. X. Zhang, “Mechanical switching of nanoscale multiferroic phase boundaries”, *Advanced Functional Materials* **25**, 3405 (2015)
21. **F. Xue**, L. Liang, Y. Gu, I. Takeuchi, S. V. Kalinin, and L.-Q. Chen, “Composition- and pressure-induced ferroelectric to antiferroelectric phase transitions in Sm-doped BiFeO₃ system”, *Applied Physics Letters* **106**, 012903 (2015)
22. **F. Xue**, Y. Gu, L. Liang, Y. Wang, and L.-Q. Chen, “Orientations of low-energy domain walls in perovskites with oxygen octahedral tilts”, *Physical Review B* **90**, 220101(R) (2014)
23. Y. Gu, **F. Xue**, S. Lei, T. T. A. Lummen, J. Wang, V. Gopalan, and L.-Q. Chen, “Monoclinic phases arising across thermal inter-ferroelectric phase transitions”, *Physical Review B* **90**, 024104 (2014)
24. H. Akamatsu, K. Fujita, T. Kuge, A. S. Gupta, A. Togo, S. Lei, **F. Xue**, G. Stone, J. M. Rondinelli, L.-Q. Chen, I. Tanaka, V. Gopalan, and K. Tanaka, “Inversion symmetry breaking by oxygen octahedral rotations in the Ruddlesden-Popper NaRTiO₄ family”, *Physical Review Letters* **112**, 187602 (2014)
25. T. Lummen, Y. Gu, J. Wang, S. Lei, **F. Xue**, A. Kumar, A. Barnes, E. Barnes, S. Denev, A. Belianinov, M. Holt, A. Morozovska, S. V. Kalinin, L.-Q. Chen, and V. Gopalan, “Thermotropic phase boundaries in classic ferroelectrics”, *Nature Communications* **5**, 3172 (2014)

26. **F. Xue**, J. J. Wang, G. Sheng, E. Huang, Y. Cao, H. H. Huang, P. Munroe, R. Mahjoub, Y. L. Li, V. Nagarajan, and L.-Q. Chen, “Phase-field simulations of ferroelectrics domain structures in $\text{PbZr}_x\text{Ti}_{1-x}\text{O}_3$ bi-layers”, *Acta Materialia* **61**, 2909 (2013)
27. L. Liang, Y. Qi, **F. Xue**, S. Bhattacharya, S. Harris, and L.-Q. Chen, “Nonlinear phase-field model for electrode-electrolyte interface evolution”, *Physical Review E* **86**, 051609 (2012)
28. L. Liang, Y. L. Li, **F. Xue**, and L.-Q. Chen, “Pressure and electric field effects on piezoelectric responses of KNbO_3 ”, *Journal of Applied Physics* **112**, 064106 (2012)
29. X. S. Gao, **F. Xue**, M. H. Qin, J.-M. Liu, B. J. Rodriguez, L.-F. Liu, M. Alexe, and D. Hesse, “Bubble polarization domain patterns in periodically ordered epitaxial ferroelectric nanodot arrays”, *Journal of Applied Physics* **110**, 052006 (2011)
30. **F. Xue**, X. S. Gao, and J.-M. Liu, “Monte Carlo simulation on the size effect in ferroelectric nanostructures”, *Journal of Applied Physics* **106**, 114103 (2009)

Manuscripts in Preparation

1. Y. Shi, **F. Xue**, and L.-Q. Chen, “Ginzburg-Landau theory of VO_2 metal-insulator transition: the electronic degrees of freedom”, (submitted to *Europhysics Letters*)
2. D. Lee, B. Chung, Y. Shi, K. Song, N. Campbell, **F. Xue**, G.-Y. Kim, S. Y. Choi, J. P. Podkaminer, T. H. Kim, P. J. Ryan, J.-W. Kim, T. R. Paudel, J.-H. Kang, J. W. Spinuzzi, D. A. Tenne, E. Y. Tsybal, M. S. Rzchowski, L.-Q. Chen, J. Lee, and C. B. Eom, “Isostructural metal-insulator transition”, (Resubmitted to *Science*)
3. **F. Xue**, N. Wang, X. Wang, Y. Ji, S.-W. Cheong, and L.-Q. Chen, “Topological dynamics of vortex-line networks in hexagonal manganites”, (submitted to *Physical Review B: Rapid Communications*, *arXiv:1705.09867*)
4. M.-G. Han, J. Li, **F. Xue**, X. Wang, J. Tao, L.-Q. Chen, S.-W. Cheong, and Y. Zhu, “Observation of vortex ordering along charged domain walls in hexagonal manganites by *in situ* arc heating and quenching”, (submitted to *Nano Letters*)
5. Y.-L. Huang, B.-C. Huang, Y.-T. Wang, **F. Xue**, J.-C. Lin, H.-J. Liu, J.-Y. Lin, C.-S. Chang, L.-Q. Chen, Y.-P. Chiu, and Y.-H. Chu, “Anisotropic superconductivity induced by periodic multiferroic domain patterns”, (in preparation)

Honors and Awards

Merit student of Jiangsu Province, 2010

Meritorious Winner in the Mathematical Contest in Modeling, 2009

Teaching Experience

Jan. 2014-Apr. 2014, Teaching Assistant of “Kinetics of Materials Processes”

Outreach Activities

- Mentor in Summer Experience in Earth and Mineral Sciences, 06/15-07/21, 2015
- Final Planning Meeting of 5-th cart-based Museum Show, 02/14/2013
- Presenter in “Arts Fest Kids Day 2012”, 07/11/2012
- Presenter in “Discovery Space Museum”, 10/22/2011