

# Haixuan Xu

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## © RESEARCH INTERESTS

**Defect evolution and interaction, radiation effects, deformation mechanism and electronic/magnetic effects on mechanical properties of structural alloys, flexoelectric effects and electromagnetic coupling, long-time atomistic simulations, on-the-fly kinetic Monte Carlo methods, materials for neuromorphic computing**

## © EDUCATION

**Ph.D.** in Materials Science and Engineering, University of Florida, Gainesville, FL, U.S. May 2010  
**M.S.** in Materials Science and Engineering, University of Florida, Gainesville, FL, U.S. August 2007  
**B.E.** in Metallic Materials Engineering, Dalian University of Technology, China June 2005

## © RESEARCH EXPERIENCE

**Assistant Professor**, Department of Materials Science and Engineering, University of Tennessee Knoxville, August 2013–present  
**Adjunct Faculty**, Department of Physics and Astronomy, University of Tennessee Knoxville, April 2018–present  
**Visiting Research Scientist**, Materials Theory Group, Oak Ridge National Laboratory (ORNL) 2013–present  
**CDP Postdoctoral Fellow**, Center of Defect Physics, Oak Ridge National Laboratory (ORNL) June 2010–July 2013

## © SELECTED HONORS AND AWARDS

**Department of Energy (DOE) Early Career Award, 2018**  
**TCE Professional Promise in Research Award, Tickle College of Engineering, UTK, 2018**  
**National Science Foundation (NSF) Early Career Award, 2017**  
**Faculty of Excellence in Research, Department of Materials Science and Engineering, UTK, 2017**  
**Faculty of Excellence in Teaching, Department of Materials Science and Engineering, UTK, 2016**  
**CDP Postdoctoral Fellowship** of Center of Defect Physics in Structural Materials at Oak Ridge National Laboratory 2010- 2013  
**National First Prize** of China Undergraduate Mathematical Contest in Modeling (CUMCM) Administered by Ministry of Education of China and China Society for Industrial and Applied Mathematics (CSIAM), 2004 and 2003  
**Meritorious Winner** of Mathematical Contest in Modeling (MCM) administered by the Consortium for Mathematics and its Applications (COMAP) of the U.S.A, 2004

## © PUBLICATIONS

1. L. Zhang, I. Bredeson, A. Birenbaum, P.R.C. Kent, V.R. Cooper, P. Ganesh, **H. Xu\***, “Oxygen Vacancy Formation Energies in PbTiO<sub>3</sub>/SrTiO<sub>3</sub> Superlattices”, *Physical Review Materials*, 2, 06449 (2018) DOI: [10.1103/PhysRevMaterials.2.064409](https://doi.org/10.1103/PhysRevMaterials.2.064409)

2. C. Zhang, P.R. Pudasaini, A. Oyedele, A. Ievlev, L. Xu, A. Haglund, J. H. Noh, A. Wong, K. Xiao, T.Z. Ward, D. Mandrus, **H. Xu**, O. Ovchinnikova, P. Rack, “Ion Migration Studies in Exfoliated 2D Molybdenum Oxide via Ionic Liquid Gating for Neuromorphic Device Applications”, *ACS Applied Materials & Interfaces*, 10, 22623 (2018) DOI: [10.1021/acsami.8b05577](https://doi.org/10.1021/acsami.8b05577)
3. T.R. Dasa, L. Hao, J. Yang, J. Liu, **H. Xu\***, “Strain Effect on Structural and Magnetic Properties of SrIrO<sub>3</sub>/SrTiO<sub>3</sub> Superlattice”, *Materials Today Physics*, 4, 43-49 (2018) DOI: [10.1016/j.mtphys.2018.02.003](https://doi.org/10.1016/j.mtphys.2018.02.003)
4. L. Hao, D. Meyers, H. Suwa, J. Yang, C. Frederick, T.R. Dasa, G. Fabbris, L. Horak, D. Kriegner, Y. Choi, J.W. Kim, D. Haskel, P. Ryan, **H. Xu\***, C.D. Batista, M.P.M. Dean, J. Liu, “Giant Magnetic Response of A Two-Dimensional Antiferromagnet”, *Nature Physics*, (2018) DOI: [10.1038/s41567-018-0152-6](https://doi.org/10.1038/s41567-018-0152-6)
5. A. Ervin, **H. Xu\***, “Mesoscale Simulations of Radiation Damage Effects in Materials: a SEAKMC Perspective”, *Computational Materials Science*, 150, 180-189 (2018) DOI: [10.1016/j.commatsci.2018.03.054](https://doi.org/10.1016/j.commatsci.2018.03.054)
6. A. Plymill, **H. Xu\***, “Flexoelectricity in ATiO<sub>3</sub> (A=Sr, Ba, Pb) Perovskite Oxide Superlattices from Density Functional Theory”, *Journal of Applied Physics*, 123, 144101 (2018) DOI: [10.1063/1.5018405](https://doi.org/10.1063/1.5018405)
7. I. Bredeson, L. Zhang, P.R.C. Kent, V.R. Cooper, **H. Xu\***, “Dimensional Control of Defect Dynamics in Perovskite Oxide Superlattices”, *Physical Review Materials*, 2, 035401 (2018) DOI: [10.1103/PhysRevMaterials.2.035401](https://doi.org/10.1103/PhysRevMaterials.2.035401)
8. H. Li, Y. Qin, Y. Yang, M. Yao, X. Wang, **H. Xu**, S.R. Phillpot, “The Evolution of Interaction between Grain Boundary and Irradiation-induced Point Defects: Symmetric Tilt GB in Tungsten”, *Journal of Nuclear Materials*, 500, 42 (2018) DOI: [10.1016/j.jnucmat.2017.12.013](https://doi.org/10.1016/j.jnucmat.2017.12.013)
9. J. Xi, B. Liu, **H. Xu**, Y. Zhang, W.J. Weber, “Determination of Gaseous Fission Product Behavior near the Cerium Dioxide Tilt Grain Boundary via First-Principles Study”, *Journal of Nuclear Materials*, 499, 377 (2018) DOI: [10.1016/j.jnucmat.2017.11.046](https://doi.org/10.1016/j.jnucmat.2017.11.046)
10. L. Casillas-Trujillo, G. Baldinozzi, M.K. Patel, **H. Xu**, K.E. Sickafus, “Comparison of Bonding and Charge Density in δ-UO<sub>3</sub>, γ-UO<sub>3</sub>, and La<sub>6</sub>UO<sub>12</sub>”, *Physical Review Materials* 1 (6), 065404 (2017) DOI: [10.1103/PhysRevMaterials.1.065404](https://doi.org/10.1103/PhysRevMaterials.1.065404)
11. L. Casillas-Trujillo, L. Xu, **H. Xu\***, “Compositional Effects on Ideal Shear Strength in Fe-Cr Alloys”, *Journal of Alloys and Compounds* 720, 466-472 (2017) DOI: [10.1016/j.jallcom.2017.05.167](https://doi.org/10.1016/j.jallcom.2017.05.167)
12. T. Chen, L. Tan, Z. Lu, and **H. Xu**, “The Effect of Grain Orientation on Nanoindentation Behavior of Model Austenitic Alloy Fe-20Cr-25Ni”, *Acta Materialia*, 138, 83-91 (2017) DOI: [10.1016/j.actamat.2017.07.028](https://doi.org/10.1016/j.actamat.2017.07.028)
13. J. Xi, **H. Xu**, Y. Zhang, W.J. Weber, “Strain Effects on Oxygen Vacancy Energetics in KTaO<sub>3</sub>”, *Physical Chemistry Chemical Physics*, 19 (8) 6364-6373 (2017) DOI: [10.1039/C6CP08315C](https://doi.org/10.1039/C6CP08315C)
14. L. Casillas-Trujillo, **H. Xu\***, J.W. McMurray, D. Shin, G. Baldinozzi, K.E. Sickafus, “Structure and Cation Ordering in La<sub>2</sub>UO<sub>6</sub>, Ce<sub>2</sub>UO<sub>6</sub>, LaUO<sub>4</sub>, and CeUO<sub>4</sub> by First Principles Calculations”, *Computational Materials Science*, 123, 201 (2016) DOI: <https://doi.org/10.1016/j.commatsci.2016.05.042>
15. D. Yi, J. Liu, S. Hsu, L. Zhang, Y. Choi, J. Kim, Z. Chen, J.D. Clarkson, C.R. Serrao, E. Arenholz, P.J. Ryan, **H. Xu**, R.J. Birgeneau, R. Ramesh, “Atomic-Scale Control of Magnetic Anisotropy via Novel Spin-Orbit Coupling Effect in La<sub>2/3</sub>Sr<sub>1/3</sub>MnO<sub>3</sub>/SrIrO<sub>3</sub> Superlattices”, *Proceedings of the National Academy of Sciences*, 113, 6397 (2016) DOI: [10.1073/pnas.1524689113](https://doi.org/10.1073/pnas.1524689113)
16. M.T. McDonnell, **H. Xu**, D.J. Keffer, “Ab Initio Molecular Dynamics Simulations of an Excess Proton in a Triethylene Glycol-Water Solution: Solvation Structure, Mechanism and Kinetics”, *The Journal of Physical Chemistry B*, 120, 5223 (2016) DOI: [10.1021/acs.jpcc.6b02445](https://doi.org/10.1021/acs.jpcc.6b02445)
17. L. Zhang, B. Liu, H. Zhuang, P.R.C Kent, V.R. Cooper, P. Ganesh, **H. Xu\***, “Oxygen Vacancy Diffusion in Bulk SrTiO<sub>3</sub> from Density Functional Theory Calculations”, *Computational Materials Science*, 118, 309 (2016) DOI: [10.1016/j.commatsci.2016.02.041](https://doi.org/10.1016/j.commatsci.2016.02.041)
18. H.L. Zhuang, L. Zhang, **H. Xu**, P.R.C Kent, P. Ganesh, V.R. Cooper, “Tunable One-Dimensional Electron Gas Carrier Densities at Nanostructured Oxide Interfaces”, *Scientific reports*, 6, 25452 (2016) DOI: [10.1038/srep25452](https://doi.org/10.1038/srep25452)

19. H.L. Zhuang, V.R. Cooper, **H. Xu**, P. Ganesh, R.G. Hennig, P.R.C. Kent, “Rashba Effect in Single-Layer Antimony Telluroiodide SbTeI”, *Physical Review B*, 92, 115302 (2015) DOI: [10.1103/PhysRevB.92.115302](https://doi.org/10.1103/PhysRevB.92.115302)
20. K. Nakashima, R.E. Stoller, **H. Xu**, “Recombination Radius of a Frenkel Pair and Capture Radius of a Self-Interstitial Atom by Vacancy Clusters in bcc Fe”, *Journal of Physics: Condensed Matter* 27, 335401, (2015) DOI: [10.1088/0953-8984/27/33/335401](https://doi.org/10.1088/0953-8984/27/33/335401)
21. L.K. Béland, Y.N. Osetsky, R.E. Stoller, **H. Xu\***, “Interstitial Loop Transformations in FeCr”, *Journal of Alloys and Compounds*, 640, 219 (2015) DOI: [10.1016/j.jallcom.2015.03.173](https://doi.org/10.1016/j.jallcom.2015.03.173)
22. **H. Xu\***, R. E. Stoller, L.K. Béland, Y. N. Osetsky, “Self-Evolving Atomistic Kinetic Monte Carlo simulations of defects in materials”, *Computational Materials Science* 100, 135, (2015) DOI: [10.1016/j.commatsci.2014.12.026](https://doi.org/10.1016/j.commatsci.2014.12.026)
23. L.K. Béland, Y. N. Osetsky, R. E. Stoller, and **H. Xu\***, “Slow Relaxation of Cascade-Induced Defects in Fe”, *Physical Review B* 91, 054108, (2015) DOI: [10.1103/PhysRevB.91.054108](https://doi.org/10.1103/PhysRevB.91.054108)
24. L.K. Béland, Y. N. Osetsky, R. E. Stoller, **H. Xu\***, “Kinetic Activation–Relaxation Technique and Self-Evolving Atomistic Kinetic Monte Carlo: Comparison of on-the-fly Kinetic Monte Carlo algorithms”, *Computational Materials Science* 100, 124, (2015) DOI: [10.1016/j.commatsci.2014.12.001](https://doi.org/10.1016/j.commatsci.2014.12.001)
25. A.V. Barashev, **H. Xu\***, R.E. Stoller, “The Behavior of Small Helium Clusters near Free Surfaces in Tungsten”, *Journal of Nuclear Materials*, 454, 421 (2014) DOI: [10.1016/j.jnucmat.2014.08.033](https://doi.org/10.1016/j.jnucmat.2014.08.033)
26. H. L. Zhuang\*, P. Ganesh\*, Valentino R. Cooper, **H. Xu**, and P.R.C. Kent, “Understanding the Interactions between Oxygen Vacancies at SrTiO<sub>3</sub> (001) Surfaces”, *Physical Review B*, 90, 064106 (2014) DOI: [10.1103/PhysRevB.90.064106](https://doi.org/10.1103/PhysRevB.90.064106)
27. B. Liu, H. Xiao, Y. Zhang, V. R. Cooper, **H. Xu**, and W.J. Weber, “Composition Dependent Intrinsic Defect Structures in SrTiO<sub>3</sub>”, *Physical Chemistry Chemical Physics*, 16, 15590, (2014) DOI: [10.1039/C4CP01510J](https://doi.org/10.1039/C4CP01510J)
28. **H. Xu\***, R.E. Stoller, Y.N. Osetsky, “Cascade Defect Evolution Processes: Comparison of Atomistic Methods”, *Journal of Nuclear Materials*, 443, 66 (2013) DOI: [10.1016/j.jnucmat.2013.07.001](https://doi.org/10.1016/j.jnucmat.2013.07.001)
29. N.J. Podraza, W. Qiu, B.B. Hinojosa, **H. Xu**, M.A. Motyka, S.R. Phillpot, J.E. Baciak, S.R. McKinstry, J.C. Nino, “Band Gap and Structure of Single Crystal BiI<sub>3</sub>: Resolving Discrepancy in Literature”, *Journal of Applied Physics*, 114, 033110 (2013) DOI: [10.1063/1.4813486](https://doi.org/10.1063/1.4813486)
30. **H. Xu\***, R.E. Stoller, Y.N. Osetsky, D. Terentyev, “Solving the Puzzle of <100> Interstitial Loop Formation in bcc Iron”, *Physical Review Letter*, 110, 265503 (2013) DOI: [10.1103/PhysRevLett.110.265503](https://doi.org/10.1103/PhysRevLett.110.265503)
31. G. Stone, D. Lee, **H. Xu**, S.R. Phillpot, V. Dierolf, “Local Probing of the Interaction between Intrinsic Defects and Ferroelectric Domain Wall in Lithium Niobate”, *Applied Physics Letter*, 102, 042905 (2013) DOI: [10.1063/1.4789779](https://doi.org/10.1063/1.4789779)
32. R.K. Behera, C.S. Deo\*, and **H. Xu**, “Effect of the Substitution of f-electron Elements on the Structure and Elastic Properties of UO<sub>2</sub>”, *Journal of Nuclear Materials*, 443, 504 (2013) DOI: [10.1016/j.jnucmat.2012.09.031](https://doi.org/10.1016/j.jnucmat.2012.09.031)
33. **H. Xu\***, Y.N. Osetsky, R.E. Stoller, “Self-Evolving Atomistic kinetic Monte Carlo: Fundamentals and Applications”, *Journal of Physics: Condensed Matter* 24,375402 (2012) DOI: [10.1088/0953-8984/24/37/375402](https://doi.org/10.1088/0953-8984/24/37/375402)
34. **H. Xu\***, Y.N. Osetsky, R.E. Stoller, “Cascade Annealing Simulations of bcc Iron using Object Kinetic Monte Carlo”, *Journal of Nuclear Materials* 423, 102 (2012) DOI: [10.1016/j.jnucmat.2012.01.020](https://doi.org/10.1016/j.jnucmat.2012.01.020)
35. **H. Xu\***, Y.N. Osetsky, R.E. Stoller, “Simulating Complex Atomistic Processes: On-the-Fly Kinetic Monte Carlo Scheme with Selective Active Volume”, *Physical Review B, Brief Reports*, 84, 132103 (2011) DOI: [10.1103/PhysRevB.84.132103](https://doi.org/10.1103/PhysRevB.84.132103)
36. D. Lee, **H. Xu**, V. Dierolf, V. Gopalan and S.R. Phillpot, “Shape of Ferroelectric Domains in LiNbO<sub>3</sub> and LiTaO<sub>3</sub> from Defect/Domain Wall Interaction”, *Applied Physics Letters* 98, 092903 (2011) <https://doi.org/10.1063/1.3560343>
37. **H. Xu**, A. Chernatynskiy, D. Lee, S.B. Sinnott, V. Gopalan, V. Dierolf and S.R. Phillpot, “Stability and Charge Transfer Levels of Extrinsic Defects in LiNbO<sub>3</sub>”, *Physical Review B* 82, 184109 (2010) DOI: [10.1103/PhysRevB.82.184109](https://doi.org/10.1103/PhysRevB.82.184109)

38. **H. Xu**, D.W. Lee, S.B. Sinnott, V. Gopalan, V. Dierolf and S.R. Phillpot, “Interactions of Defects and Domain Walls in LiNbO<sub>3</sub> – Insights from Simulation”, IOP Conf. Ser.: MSE. 15, 012003 (2010) DOI: [10.1088/1757-899X/15/1/012003](https://doi.org/10.1088/1757-899X/15/1/012003)
39. **H. Xu**, D. Lee, S.B. Sinnott, V. Gopalan, V. Dierolf and S.R. Phillpot, “Structure and Diffusion of Intrinsic Defect Complexes in LiNbO<sub>3</sub> from DFT Calculations”, J. Phys.: Condens. Matter 22, 135002 (2010) DOI: [10.1088/0953-8984/22/13/135002](https://doi.org/10.1088/0953-8984/22/13/135002)
40. **H. Xu**, R.K. Behera, Y. Wang, F. Ebrahimi, E.D. Wachsman, S.B. Sinnott and S.R. Phillpot, “A Critical Assessment of Interatomic Potentials for Ceria with Application to its Elastic Properties”, Solid State Ionics 181, 551 (2010) DOI: [10.1016/j.ssi.2010.02.023](https://doi.org/10.1016/j.ssi.2010.02.023)
41. D. Lee, **H. Xu**, V. Dierolf, V. Gopalan and S.R. Phillpot, “Structure and Energetics of Ferroelectric Domain Walls in LiNbO<sub>3</sub> from Atomic-Level Simulations”, Physical Review B 82, 014104 (2010) DOI: [10.1103/PhysRevB.82.014104](https://doi.org/10.1103/PhysRevB.82.014104)
42. **H. Xu**, D. Lee, S.B. Sinnott, V. Gopalan, V. Dierolf and S.R. Phillpot, “Structure and Energetics of Er Defects in LiNbO<sub>3</sub> from First Principles and Thermodynamic Calculations”, Physical Review B 80, 144104 (2009) DOI: [10.1103/PhysRevB.80.144104](https://doi.org/10.1103/PhysRevB.80.144104)
43. D. Lee, R. K. Behera, P. Wu, **H. Xu**, S.B. Sinnott, S.R. Phillpot, L. Q. Chen, and V. Gopalan, “Mixed Bloch-Néel-Ising Character of 180° Ferroelectric Domain Walls”, Physical Review B, Rapid Communication, 80, 060102(R) (2009) <https://doi.org/10.1103/PhysRevB.80.060102>
44. **H. Xu**, D. Lee, J. He, S.B. Sinnott, V. Gopalan, V. Dierolf and S.R. Phillpot, “Stability of Intrinsic Defects and Defect Clusters in LiNbO<sub>3</sub> from Density Functional Theory Calculations”, Physical Review B 78, 174103 (2008) DOI: [10.1103/PhysRevB.78.174103](https://doi.org/10.1103/PhysRevB.78.174103)
45. M. He, B. Li, **H. Xu**, L.D. Luo, “A Three-Opinion SZNAJD Model with Limited Persuasion and Its Applications”, International Journal of Modern Physics C 16, 1449 (2005) DOI: [10.1142/S0129183105008096](https://doi.org/10.1142/S0129183105008096)
46. M. He, **H. Xu**, Q. Sun, “Opinion Evolution on a Scale-Free Network with Leaders”, International Journal of Modern Physics C 15, 947 (2004) DOI: [10.1142/S012918310400639X](https://doi.org/10.1142/S012918310400639X)

## © PUBLICATIONS UNDER REVIEW OR IN PREPARISON

1. L. Casillas-Trujillo, A.S. Ervin, L. Xu, A. Barashev, **H. Xu\***, “Point Defect Interaction with Dislocations in bcc Iron”, Physical Review Materials, accepted
2. Z. Lu, L. Xu, T. Chen, L. Tan and **H. Xu\***, “Interactions between Displacement Cascade and Dislocation and Their Influences on Peierls Stress in Fe-20Cr-25Ni alloys”, Journal of Nuclear Materials, under revision
3. V.R. Cooper, H.L. Zhuang, L. Zhang, P. Ganesh, **H. Xu**, and P.R.C. Kent, “Anomalous Dielectric Response at Intermixed Oxide Heterointerfaces”, submitted to npj Computational Materials, under review
4. T. Chen, Y. Yang, L. He, B. Tyburska-Püschel, K. Sridharan, **H. Xu**, L. Tan, “Enhanced Diffusion of Cr in 20Cr-25Ni Type Alloys under Proton Irradiation at 670 °C”, in progress, Journal of Nuclear Materials.
5. T. Chen, L.F. He, J. Burns, Y. Wu, C. Knight, K. Sridharan, **H. Xu**, L. Tan, “Microstructure and Mechanical Properties of ATR-irradiated NF709 Stainless Steel”, in progress, Journal of Nuclear Materials.

## © COMPUTING ALLOCATIONS

1. Project ID TG-DMR170112, 1.347 million SUs on Comet & 1.572 million SUs on Bridges at Extreme Science and Engineering Discovery Environment (XSEDE), Jan 2018 – Dec 2018.
2. Project ID MAT173, 2 million core hours on Titan & 2500 node hours on Rhea at Oak Ridge Leadership Computing Facility (OLCF), Oct 2017 – Oct 2018.

3. Project ID TG-DMR170020, 50,000 SUs on Comet & 50,000 SUs on Bridges & 1560 SUs on Stampede2 at Extreme Science and Engineering Discovery Environment (XSEDE), Mar 2017 – Feb 2018.
4. Project ID UT-TENN0112, 6 million SUs on National Institute of Computational Sciences (NICS), 2014-2016

## © INVITED PRESENTATIONS

1. (Keynote) **H. Xu**, “Mesoscale Simulations of Interaction between Point Defect and Dislocation in bcc Iron using SEAKMC”, Chinese Materials Conference, Yinchuan, China, July 2017
2. **H. Xu**, “Interactions between Point Defects and Dislocations in bcc Iron using SEAKMC”, 2017 International Symposium on Multiscale Modelling and Simulation of Materials, Shenyang, China, July 2017
3. **H. Xu**, “Spin-orbit Coupling Effects in 5d Metal Oxide Superlattices from DFT Calculations”, 12th Pacific Rim Conference on Ceramic and Glass Technology, Waikoloa, HI, May 2017
4. **H. Xu**, “Defect Stability and Transport in SrTiO<sub>3</sub>/PbTiO<sub>3</sub> Superlattice from Density Functional Theory”, 41th International Conference and Expo on Advanced Ceramics and Composites (ICACC 2017), Daytona Beach, FL, January 2017
5. **H. Xu**, “Defect Evolution in Structural Materials from SEAKMC Simulations: Opportunities and Challenges”, Bridging-Time Scale Techniques and their Applications in Atomistic Computational Science, Dresden, Germany, Sep 2016
6. **H. Xu**, “Long-Term Defect Evolution in Iron from SEAKMC Simulations”, TMS Annual Meeting, Nashville, TN, U.S. Feb 2016
7. **H. Xu**, “Defect Properties in Perovskite Oxide Superlattices from Density Functional Theory”, 40th International Conference and Expo on Advanced Ceramics and Composites (ICACC 2016), Daytona Beach, FL, January 2016
8. **H. Xu**, “Long-Term Defect Evolution in Iron-based Alloys from SEAKMC Simulations”, 2015-International Symposium on Multiscale Modeling and Simulation of Materials, Beijing, China, July 2015
9. **H. Xu**, “Defect Transport in Perovskite Oxide Superlattice from Density Functional Theory”, 11th International Conference on Ceramic Materials and Components for Energy and Environmental Applications, Vancouver, Canada, July 2015
10. (Keynote) **H. Xu**, “Long-Term Defect Evolution in Materials using on-the-fly Kinetic Monte Carlo”, Enabling Methods for Materials Innovation: From Quantum to Mesoscale Workshop, Gainesville, FL, 2015
11. **H. Xu**, G.M. Stocks, and Y.N. Osetsky, R.E. Stoller, “Defect Interaction and Evolution in Iron and Its-based Alloys”, 7th International Conferences on Multiscale Materials Modeling (MMM 2014), Berkeley, CA, 2014
12. **H. Xu**, “Radiation Induced Defect Evolution and Their Influence in Mechanical Properties of Iron- based Structure Materials”, 17th U.S. National Congress on Theoretical & Applied Mechanics, East Lansing, MI, 2014
13. **H. Xu**, Y.N. Osetsky, and R.E. Stoller, “Self-Evolving Atomistic Kinetic Monte Carlo: Development and Application”, Conference on Computational Physics (CCP), Gatlinburg, TN, 2011

## © CONTRIBUTED PRESENTATIONS

1. A.S. Ervin, L. Casillas-Trujillo, **H. Xu**, “Dislocation Loop Bias in bcc Fe”, TMS, Phoenix, AZ March 2018
2. T. Dasa, L. Hao, J. Liu, **H. Xu**, “Strain effects on Structural and Magnetic properties of SrIrO<sub>3</sub>/SrTiO<sub>3</sub> superlattice”, American Physics Society (APS) March meeting, Los Angeles, CA, March 2018
3. L. Hao, D. Meyers, H. Suwa, J. Yang, C. Frederick, T. Dasa, G. Fabbris, L. Horak, D. Kriegner, Y. Choi, J. W. Kim, D. Haskel, P. Ryan, **H. Xu**, C. Batista, M. Dean, J. Liu, “Capturing the Hidden Symmetry in Layered Iridate Heterostructures”, American Physics Society (APS) March meeting, Los Angeles, CA, March 2018
4. J. Yang, L. Hao, J. Liu, D. Meyers, M. Dean, C. Frederick, L. Horak, D. Kriegner, Y. Choi, J. W. Kim, D. Haskel, T. Dasa, **H. Xu**, P. Ryan, “Strain Control of Electric and Magnetic Properties in Iridate Heterostructures”, American

Physics Society (APS) March meeting, Los Angeles, CA, March 2018

5. V. Cooper, H. Zhuang, L. Zhang, P. Ganesh, **H. Xu**, P.R.C. Kent, “Anomalous Dielectric Response at Oxide Heterointerfaces”, American Physics Society (APS) March meeting, Los Angeles, CA, March 2018
6. **H. Xu**, “Integrated Computational and Experimental Study of Radiation Damage Effects in Alloy 709”, Spring MRS meeting, Phoenix, AZ, US, April 2017
7. **H. Xu**, “Dynamics of Interaction between Point Defects and Dislocations in bcc Iron using SEAKMC Simulations”, TMS Annual Meeting, San Diego, CA, U.S. Feb 2017
8. L. Casillas-Trujillo, G. Baldinozzi, M. K. Patel, **H. Xu**, K.E. Sickafus, “Comparison of Bonding and Charge Density in delta-UO<sub>3</sub>, gamma-UO<sub>3</sub>, and La<sub>6</sub>UO<sub>12</sub>”, eMRS Fall Meeting, Warsaw, Poland, September 2017
9. L. Casillas-Trujillo, **H. Xu**, “Dynamics of Interactions between Point Defects and Dislocations in bcc Iron”, MRS spring meeting, Phoenix, AZ, April 2017
10. L. Casillas-Trujillo, G. Baldinozzi, **H. Xu**, K.E. Sickafus, “Charge Distribution and Chemical Bonds in UO<sub>3</sub> polymorphs”, MRS spring meeting, Phoenix, AZ, March 2016
11. L. Casillas-Trujillo, K.E. Sickafus, **H. Xu**, “Structure and Cation Ordering of ULa<sub>2</sub>O<sub>6</sub>, ULaO<sub>4</sub>, UCe<sub>2</sub>O<sub>6</sub>, UCeO<sub>4</sub> by First Principles Calculations”, CMCEE, Vancouver, Canada, June 2015
12. V.R. Cooper, L. Zhuang, P. Ganesh, **H. Xu**, P.R.C. Kent, “Interfacial Intermixing in  $\delta$ -doped Oxide Superlattices”, American Physics Society (APS) March meeting, San Antonio, TX, March 2015
13. **H. Xu**, L. Casillas-Trujillo, “Ideal Shear Strength of Iron-based Alloys from First Principles Calculations”, Spring MRS Meeting, San Francisco, CA, 2015
14. **H. Xu**, “Flexoelectricity in Perovskite Oxide Superlattices from Density Functional Theory”, The International Chemical Congress of Pacific Basin Societies, Honolulu, Hawaii, USA, December 2015
15. **H. Xu**, R.E. Stoller, and Y.N. Osetsky, “Defect Interaction in Iron and Iron-based Alloys”, APS March Meeting, Denver, CO, 2014
16. **H. Xu**, R.E. Stoller, and G. M. Stocks, “The Mechanism of <100> Interstitial Formation in bcc Iron”, MRS Fall Meeting, Boston, MA, 2013
17. **H. Xu**, R.E. Stoller, and Y.N. Osetsky, “Defect Evolution and Interaction of Helium in bcc Metals under Fusion and Fission Environment”, 16th International Conference on Fusion Reactor Materials (ICFRM 16), Beijing, China, 2013
18. **H. Xu**, R.E. Stoller, and G. M. Stocks, “Magnetic Evolution of the <100> Interstitial Formation Process in bcc Iron”, APS Annual Meeting, Baltimore, MD, 2013
19. **H. Xu\***, R. E. Stoller, Y. N. Osetsky, B. C. Larson, G. M. Stocks, V. McCreary, I. M. Robertson, “The <100> Interstitial Loop Formation Process in bcc Iron”, EFRC PI Meeting, Washington D.C. 2013
20. **H. Xu**, Y.N. Osetsky, and R.E. Stoller, “Annealing Simulation of Radiation Damage Using Self-Evolving Atomistic Kinetic Monte Carlo”, MRS Fall Meeting, Boston, MA, 2012
21. **H. Xu**, Y.N. Osetsky, and R.E. Stoller, “Self-Evolving Atomistic Monte Carlo Method (SEAKMC): Development and Applications”, COSIRES, Santa Fe, NM, 2012
22. **H. Xu**, Y.N. Osetsky, and R.E. Stoller, “Development and Application of a New Atomistic Monte Carlo Method for Defect Evolution”, EFRC Science Review, Denver, CO, 2012
23. **H. Xu**, Y.N. Osetsky, S. Golubov and R.E. Stoller, “Kinetics of Vacancy and Interstitial Defects Absorption by Edge Dislocations: a Kinetic Monte Carlo Study”, 15th International Conference on Fusion Reactor Materials (ICFRM-15), Charleston, SC, 2011
24. **H. Xu**, Y.N. Osetsky, and R.E. Stoller, “Kinetic Monte Carlo Simulations of Defect Evolution Produced by Primary Damage in bcc Iron”, ASTM International, 25th Symposium on Effects of Radiation on Nuclear Materials, Los Angeles, CA, 2011
25. **H. Xu**, Y.N. Osetsky, and R.E. Stoller, “Primary Damage Evolution in bcc Fe using Kinetic Monte Carlo Simulations”, Science for Our Nation’s Energy Future: Energy Frontier Research Center Summit and Forum,

Washington D.C, 2011

26. **H. Xu**, Y.N. Osetsky, and R.E. Stoller, “Point Defect Evolution Produced by Primary Damage in bcc Iron using Kinetic Monte Carlo Simulations”, MRS Spring Meeting, San Francisco, CA, 2011
27. **H. Xu**, Y.N. Osetsky, and R.E. Stoller, “Development and Application of a New Self-Evolving Atomistic Kinetic Monte Carlo (SEAKMC) Method”, IEA-Workshop, LLNL, Livermore, CA, 2011
28. **H. Xu**, D. Lee, S. B. Sinnott, V. Gopalan, V. Dierolf and S. R. Phillpot, “Defects and Domain Walls in LiNbO<sub>3</sub>: Insights from Microscopic Simulation”, TMS Annual Meeting, San Francisco, CA, 2009
29. **H. Xu**, D. Lee, S.B. Sinnott, V. Gopalan, V. Dierolf, and S.R. Phillpot, “Intrinsic Defects and Defect Clusters in LiNbO<sub>3</sub> From Density Functional Theory and Thermodynamic Calculations”, Gordon Research Conference: Time-Dependent Density Functional Theory, New London, NH, 2009
30. **H. Xu**, R.K. Behera, Y. Wang, F. Ebrahimi, S.B. Sinnott, E.D. Wachsman, and S.R. Phillpot, “Molecular Dynamics Simulations of Diffusion and Mechanical Properties in Ceria-Based Electrolytes”, MRS Fall Meeting, Boston, MA, 2008
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32. **H. Xu**, R.K. Behera, Y. Wang, F. Ebrahimi, E. D. Wachsman, S.B. Sinnott and S. R. Phillpot, “Kinetics and Mechanisms of Oxygen Diffusion in Ceria-Based Electrolytes by Molecular Dynamics Simulations”, 32nd International Conference & Exposition on Advanced Ceramics & Composites (ICACC), Daytona, FL, 2008
33. **H. Xu**, D. Lee, S.B. Sinnott, V. Gopalan, V. Dierolf and S.R. Phillpot, “Stability of Point Defects in LiNbO<sub>3</sub> using Density Functional Theory”, MRS Fall Meeting, Boston, MA, 2007
34. **H. Xu**, R.K. Behera, Y. Wang, F. Ebrahimi, E.D. Wachsman S.B. Sinnott and S.R. Phillpot, “Atomic Study of Ceria-Based Electrolytes”, Gordon Research Conference: Solid State Studies in Ceramics, Andover, NH, 2007
35. **H. Xu**, R.K. Behera, Y. Wang, F. Ebrahimi, E.D. Wachsman, S.B. Sinnott and S.R. Phillpot, “Mechanical Properties of Ceria-Based Systems using MD Simulations”, 31st International Conference & Exposition on Advanced Ceramics & Composites (ICACC), Daytona, FL, 2007

## © TEACHING EXPERIENCE

**MSE 360/367 Principles of Ceramics** (Fall 2014: 3.54/5, Fall 2015: 4.11/5)

**MSE 613 Modeling and Simulations in Materials Science and Engineering** (Spring 2015: 4.54/5, Spring 2017: 4.5/5)

**MSE 513 Thermodynamics** (Spring 2016: 4.45/5, Fall 2016: 4.75/5, Fall 2017: 4.71/5)

**Postdoctoral Researcher Supervisor:** Dr. Lipeng Zhang (2014-2016, now Faculty at Beijing University of Chemical Technology), Zizhe Lu (2016-2018, now research scientist at TCL), Tamene Dasa (2017- )

**Graduate Student Supervisor:** Luis Casillas-Trujillo (Ph.D 2014-2017, University of Linköping at Sweden), Liubin Xu (Ph.D 2015-), Andrew Ervin (Ph.D 2017-), Ziang Yu (Ph.D 2018-), Jaswanth Bommidi (Ph.D 2018-), Andrew Lubimtsev (M.S. 2016-) Xianzhe Wu (M.S 2014-2015), Eli Barlow (M.S with Prof. Rawn, 2013-2014)

**Undergraduate Student Supervisor:** Austin Plymill (2014-2016, now at Northwestern University), Dylan Dozier (2015-2017), Christopher Walker (2015-2018, will join Texas A&M University at Fall 2018), Vincenzo Musico (2018-)

**Visiting Students and Scholars:** Shiyao Qin (Beihang University, China), Jun Chai (Beihang University, China), Jiannan Hao (Beihang University, China), Sho Hayakawa (Tokyo University, Japan), Fredric Granberg (University of Helsinki, Finland), Dan Han (East China Normal University, China)

**Thesis and Qualify Exam Committee:** Jingxuan Ge, Haoling Jia, Elijah Duncan Barlow, Chao Pu, Uk Huh, Josh Arnold, Bernadette Cladek, Diana Orozco, Ali Yousefzadi Nobakht

## © PROFESSIONAL ACTIVITIES

**Member** Materials Research Society (MRS); American Physical Society (APS); The Mineral, Metals, and Materials Society (TMS), American Ceramic Society (ACerS)

**Committee Member** of TMS Nuclear Materials Committee, TMS Computational Materials Science and Engineering Committee, TMS Mechanical Behavior of Materials Committee

## © REVIEWER & ORGANIZER

**Reviewer for Funding Agencies:** U.S National Science Foundation (NSF) CMMI MEP, NSF DMR CMMT, U.S. Department of Energy (DOE) Nuclear Energy University Program (NEUP), DOE Office of Science, Swiss National Science Foundation,

**Reviewer for Journals:** Nature, Nature Communications, Physical Review Letters, Progress in Materials Science, Physical Review Materials, Acta Materialia, Scripta Materialia, Physical Review B, Physical Chemistry Chemical Physics, Scientific Reports, Journal of Applied Physics, Philosophical Magazine, Journal of Nuclear Materials, Computational Materials Science, Journal of Physics: Condensed Matter, Materials Letters, Journal of Materials Chemistry A, Inorganic Chemistry, Journal of Materials Research, Journal of Applied Crystallography, Intermetallics, Journal of American Ceramic Society, etc

### **Session Chair:**

- Symposium of “Virtual Materials (Computational) Design and Ceramic Genome” at 41th International Conference and Expo on Advanced Ceramics and Composites 2017
- Symposium of “Advances in Materials, Experiments, and Modelling for Nuclear Energy” at Spring MRS 2017
- Symposium of “Nuclear Materials” at Chinese Materials Research Society 2017
- Symposium of “Computational Materials Engineering for Nuclear Reactor Applications” at TMS Annual Meeting 2016
- Symposium of “Virtual Materials (Computational) Design and Ceramic Genome” at 40th International Conference and Expo on Advanced Ceramics and Composites 2016
- Symposium of “Structural Materials in Nuclear Reactors: Evolution of Radiation-Induced Defects in BCC Metals” at Spring MRS 2015
- Symposium of “Method development to bridge the time and space scale gap in irradiation damage simulations” at International Conferences on Multistate Materials Modelling (MMM 2014)

### **Organizer:**

- Co-organizer of “Virtual Materials (Computational) Design and Ceramic Genome” Symposium at 42th International Conference and Expo on Advanced Ceramics and Composites 2018
- Organizer of “Computational Materials Science and Engineering for Nuclear Energy” Symposium at TMS meeting 2018
- Co-organizer of “Advances in Materials, Experiments, and Modelling for Nuclear Energy” symposium at Spring MRS meeting 2017
- Co-organizer of “Ceramic Modelling” Symposium at 41th International Conference and Expo on Advanced Ceramics and Composites 2017
- Co-organizer of 26th annual Fundamental Physics of Ferroelectrics and Related Materials Workshop 2015



## © DEPARTMENT AND UNIVERSITY SERVICE

- Member of Departmental Graduate Committee
- Member of Departmental Strategic Planning Committee
- Member of Departmental Work Load Committee
- Member of Departmental Faculty Search Committee
- Member of College Graduate Council
- Heavily involved in graduate students' recruitment events