AYANA GHOSH

Computational Sciences & Engineering Division, Oak Ridge National Laboratory, TN, USA, 37831
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PRESENT POSITION

R&D Staff Scientist **03/2023 – Present**
Oak Rige National Laboratory - Computational Sciences & Engineering Division – Oak Ridge, TN, USA

EDUCATION

Postdoctoral Research Associate - Oak Ridge National Laboratory **09/2020-02/2023**
Computational Science & Engineering Division – Oak Ridge, TN, USA
Mentors: Dr. Maxim Ziatdinov (ORNL), Prof. Sergei V. Kalinin (UTK)
Focus: Functional Materials, Machine Learning Workflows for Theory-Experiment Integration, Atomistic Simulations

Doctor of Philosophy (PhD) - Materials Science & Engineering **01/2016 – 08/2020**
University of Connecticut - Department of Materials Science & Engineering – Storrs, CT, USA
Advisors: Prof. Serge M. Nakhmanson, Dr. Jian-Xin Zhu, Prof. S. Pamir Alpay
Thesis: Predicting Materials Behavior with Atomistic Simulations and Machine Learning

Bachelor of Science (BS, Honors) - Physics, Abstract Mathematics **09/2011 – 05/2015**
University of Michigan - Flint, MI, USA

SUMMARY OF SCHOLARLY CONTRIBUTIONS

Refereed Journal & Conference Papers: **46**, Citations: **1018**, h-index: **18**, Formally Invited Presentations: **32**

RESEARCH EXPERTISE

- Modeling advanced materials using atomistic simulations and AI/ML methods
- Materials systems: oxides, metals, semi-metals, polymers, and molecular crystals
- Integration of theory with experiments
- AI/ML for physical systems analysis, causal models, explainability and uncertainty quantification
- Ensemble methods, reinforcement learning, applications in quantum computing

AWARDS

- Invited to Science and Technology in Society forum - Young Leaders Program **2025**
- ORNL Director's Award for Outstanding Individual Accomplishment in Science & Technology **2024**
- Early Career Research Accomplishment, UT-Battelle ORNL Awards **2024**
- Early Discovery Award, American Ceramic Society - Basic Science Division **2024**
- People's Choice for Best Project, Office of the Laboratory Director's LDRD Poster Fair **2024**
- Travel Award for the Microscopy & Microanalysis Meeting **2024**
- Travel Award for the SIAM Conference on Mathematical Aspects of Materials (MS24) **2024**
- Special Performance Award for Extraordinary Individual Effort, CSED, ORNL **2024–2021**
- Travel fellowship for 2023 Career Mentoring Workshop organized by Computing Research Association **2023**
- Rising Star in Computational Materials Science, Sandia National Laboratories **2022**
- Best Student Poster Presentation Award, Electronic Materials and Applications, ACerS Meeting **2020**
- Doctoral Dissertation Fellowship, Doctoral Student Travel Fellowship, UConn **2020**
- Phi Kappa Phi John Tanaka Graduate Student Award, UConn **2019**
- 1st Place at 5th Annual Graduate Poster Competition, MSE, School of Engineering, UConn **2019**
- Brian D. Proffer Student Excellence Award, UM-Flint **2015**

- Student Involvement and Leadership Emerging Award, UM-Flint **2015**
- Volunteer Service Awards, UM-Flint **2015**
- Scholarships: David G. Zick, Freeman International Student, A. J. Trela Honors, International Center Freshman, Science & Technology, International Institute of Foreign National, UM-Flint **2011 – 2015**

MEDIA COVERAGE

- UConn Featured Alumni, April 2025
- ORNL News on Director's Awards, November 2024
- ORNL News on ACerS recognition, September 2024
- ORNL cover story on cation ordering, May 2023
- Story in phys.org, May 2023
- Featured Alumna of UM-Flint, October 2020
- UConn MSE News on Publication being in Top 100 the most downloaded papers on Physics, April 2020
- UConn MSE News on EMA conference, March 2020
- UConn MSE News and IMS Newsletter on Phi Kappa Phi Fellowship Award, April 2019
- UConn MSE News on Crystallization Propensity Project , April 2019

RESEARCH EXPERIENCES

Graduate Research Intern - Los Alamos National Laboratory **2016-2019**
Theoretical Division, MPA-CINT, Los Alamos, NM

- **Mentor:** Dr. Jian-Xin Zhu
- **DFT and Machine Learning**: Performed computations and built ML frameworks to estimate electronic, magnetic and polar properties of inorganic perovskites, and actinides.

Graduate Research Assistant - New Mexico State University **06/2015 – 12/2015**
Department of Physics- Las Cruces, NM

- **Advisors:** Dr. Stefan Zollner
- **Modeling multiferroic materials**: Performed characterization measurements for multiferroic materials and participated in theoretical modeling of corresponding magnetoelectric properties.

Undergraduate Research Intern - University of Nebraska-Lincoln **06/2014 – 08/2014**
Diocles Extreme Light Laboratory - Department of Physics, Lincoln, NE

- **Advisors:** Dr. Donald Umstadter, Dr. Gregory Golovin, Dr. Sudeep Banerjee
- **Interferometry and Image Reconstruction**: Performed comparative analysis of phase reconstructions, density profile of gas jets yielded using Mach-Zender and Nomarski interferometers.

Undergraduate Research Intern - New Mexico State University **05/2013 – 08/2013**
Department of Physics, Las Cruces, NM

- **Advisor:** Dr. Stefan Zollner
- **Modeling Semiconductor materials:** Built theoretical models to explain strain due to lattice mismatch and thermal expansion, optical properties using second derivative analysis.

PROFESSIONAL ACTIVITIES & OUTREACH

- Mentor for Assistant Professor at the University of Virginia via Growing External Mentoring Support (GEMS) program, 2025–Present

- Session Chair at Machine Learning in Chemical and Materials Sciences, 2025
- Selection Committee Member for Early Discovery Award by American Ceramics Society, Basic Science Division, 2025-2028
- Session Chair at Smoky Mountains Computational Sciences and Engineering Conference 2024
- Organizing Committee Member for "Scalable Machine Learning and Generative AI for Materials Design" Session at The Platform for Advanced Scientific Computing (PASC) Conference 2024
- Organizing Committee Member for AI4Mat workshop at University of Vienna 2024
- Guest editor for MRS Advances on Challenges and Opportunities in Materials by Design
- Reviewer for npj Comput. Mater., Phys. Rev. B, Phys. Rev. Mater., Phys. Rev. Research, APL Mater., Comput. Condens. Matter, J. Phys. Chem., ACS Nano, Front. Nanosci.
- Session Chair AI and Materials III, APS March Meeting 2023
- Proposals Reviewer & Judge at New Mexico Supercomputing Challenge 2018
- Member of Materials Research Society, American Physical Society, $\Phi K \Phi$ Honors Society, $\Sigma\Pi\Sigma$, Alumni of University of Michigan, University of Connecticut, John Lof Leadership Academy
- Mentor and Co-advisor for 4 undergraduate students (UConn, SRMIST), 3 PhD students (SRMIST), 2021–Present
- Workshops Presenter on Introduction to Materials Science at NM Tech Trek Event organized by American Association of University Women and Challenge Kickoff organized by New Mexico Supercomputing Challenge 2018
- Volunteer for STEM Recruiting event at Western Connecticut State University, Connecticut Invention Convention, Connecticut Science Olympiad, Hiring Fair hosted by the Connecticut Technology Council, 2016–2019
- Undergraduate Admissions Ambassador, International Student Ambassador, Teaching Assistant, Supplemental Instructor, Blog Writer, Media Assistant at UM-Flint, 2011–2015
- Poster Judge at Undergraduate Posters Session at American Physical Society March Meeting 2014

PROPOSALS (Principal Investigator)

- Early Career at ORNL (funding of $300K):
  "Causal AI framework for unconventional heterostructures" **2025–27**
- SUMMIT plus proposal at ORNL (computational resources of 250k node hours):
  "Domain dynamics of ferroelectric heterostructures at large scale using causal-informed scientific machine learning and atomistic simulations" **2023–24**
- LDRD-SEED proposal at ORNL (funding of $190K):
  "Causal machine learning for predictive materials design" **2023–24**
- CNMS-ORNL User Proposal: "A comprehensive study of functional mode coupling in real materials guided by neural networks and first-principles computations" **2021–23**
- CINT-LANL User Proposal: "A data-driven approach to study magnetic interactions in 2D systems" **2021–23**

PUBLICATIONS

Total Citations (Google Scholar): 1018, *h*-index: 18, *corresponding author **2015 – Present**

Submitted/under review in peer-reviewed journals

4. M. Shaikh, A. Ghosh* and S. Ghosh *Polar and Electronic Phase Control through Interacting Structural Modes* (2025).

3. A. Ghosh*, P. Gayathri, S. Buvaneswaran and S. Ghosh *Causal reasoning for controlling polarization switching in hybrid improper ferroelectrics* (2025).

2. S. Bagchi, A. Biswas, P.V. Balachandran, A. Ghosh* and P Ganesh, *Towards" on-demand" van der Waals epitaxy with hpc-driven online ensemble sampling*, arXiv:2504.05539 (2025).

1. A. Ghosh*, M. Ziatdinov, and S. V. Kalinin, *Active Deep kernel learning of molecular functionalities: Realizing dynamic structural embeddings*, arXiv:2403.01234 (2025).

Published in peer-reviewed journals

46. M. G. Boebinger, A. Ghosh, K. M. Roccapriore, S. Misra, K. Xiao, S. Jesse, M. Ziatdinov, S. V. Kalinin, and R. R. Unocic, *Exploring electron-beam induced modifications of materials with machine-learning assisted high temporal resolution electron microscopy*, npj Comput. Mater. **10**, 260 (2024).

45. A. Ghosh* and S. Ghosh, *Mapping causal pathways with structural modes fingerprint for perovskite oxides*, Mach. Learn.: Sci. Technol. **5**, 045014 (2024). *In focus issue on ML and the Physical Sciences.*

44. G. Saranathan, A. Ghosh*, et al., *Active learning surrogates for integrating electron microscopy and computational insights from simulations in autonomous experiments*, Proc. of the SC '24 Workshops of The Int. Conf. on High Performance Comput., Network, Storage, and Analysis (2024).

43. Z. Fox and A. Ghosh*, *Active causal learning for decoding chemical complexities with targeted interventions*, Mach. Learn.: Sci. Technol. **5**, 035056 (2024). *In focus issue on Explainable Machine Learning in Sciences.*

42. M. G. Boebinger, D. E. Yilmaz, A. Ghosh, S. Misra, T. S. Mathis, S. V. Kalinin, S. Jesse, Y. Gogotsi, A. C.T. van Duin, and R. R. Unocic, *Direct Fabrication of Atomically Defined Pores in MXenes*, Small Methods **8**, 2400203 (2024).

41. A. Ghosh*, P. Gayathri, M. Shaikh, and S. Ghosh, *Structural mode coupling in perovskite oxides using hypothesis-driven active learning*, J. Phys. Mater. **7**, 025014 (2024). *Featured in Women's Perspectives in Computational Materials Science.*

40. S.V. Kalinin, M. Ziatdinov, M. Ahmadi, A. Ghosh, K. Roccapriore, Y. Liu, and R. K. Vasudevan, *Designing workflows for materials characterization*, Appl. Phys. Rev. **11**, 011314 (2024).

39. G. Palanichamy, S. Ghosh, and A. Ghosh*, *Predictive design of hybrid improper ferroelectric double perovskite oxides*, Chem. Mater. **36**, 2 (2024). *Featured as front cover of journal.*

38. A. Ghosh*, *Towards physics-informed explainable machine learning and causal models for materials research*, Comput. Mater. Sci. **233**, 112740 (2024).

37. A. N. Morozovska, E. A. Eliseev, Y. Liu, K. P. Kelley, A. Ghosh, Y. Liu, J. Yao, N. V. Morozovsky, A. L. Kholkin, Y. M. Vysochanskii, and S. V. Kalinin, *Bending-induced isostructural transitions in ultrathin layers of van der Waals ferrielectrics*, Acta Materialia, **263**, 119519 (2024).

36. G. Saranathan, M.Foltin, A.Tripathy, M. Ziatdinov, A. M. J. Koomthanam, S. Bhattacharya, A. Ghosh et al., *Towards FAIR Workflows for Federated Experimental Sciences*, IEEE Conference on Artificial Intelligence (CAI) (2024),

35. Z. Fox and A. Ghosh*, *Active Causal Machine Learning for Molecular Property Prediction*, NeurIPS Workshop (2023).

34. M J Swamynadhan, A. Ghosh, and S. Ghosh, *Design of high polarization low switching barrier hybrid improper ferroelectric perovskite oxide superlattices*, Mater. Horiz. **10**, 5942 (2023).

33. S. V. Kalinin, D. Mukherjee, K. Roccapriore, B. J. Blaiszik, A. Ghosh, M. A. Ziatdinov, A. Al-Najjar, C. Doty, S. Akers, N. S Rao, J. C Agar, S. R Spurgeon, *Machine learning for automated experimentation in scanning transmission electron microscopy*, npj Comput. Mater. **9**, 227 (2023).

32. A. Ghosh*, D. P. Trujillo, S. Hazarika, E. Schiesser, M. Swamynathan, S. Ghosh, J.-X. Zhu, and S. Nakhmanson, *Identification of novel organic polar materials: A machine learning study with importance sampling*, APL Mach. Learn. **1**, 046115 (2023).

31. G. Saranathan, M. Foltin, A. Tripathy, M. Ziatdinov, A. M. J. Koomthanam, S. Bhattacharya, A. Ghosh, K. Roccapriore, S. R. Sukumar, and P. Faraboschi, Proc. of Int. Conf. High Perform. Comput. Netw. Storage Anal. *Towards Rapid Autonomous Electron Microscopy with Active Meta-Learning* (2023).

30. Y. Liu, A. N Morozovska, A. Ghosh, K. P Kelley, E. A Eliseev, J. Yao, Y. Liu, and S. V. Kalinin, *Stress and curvature effects in layered 2D ferroelectric $CuInP_2S_6$*, ACS Nano **17**, 22004 (2023).

29. G. Palanichamy, M. J. Swamynadhan, M. Shaikh, A. Ghosh*, and S. Ghosh, *Switching of Hybrid Improper Ferroelectricity in Oxide Double Perovskites*, Chem. Mater. **35**, 6612 (2023).

28. A. N. Morozovska , E. A. Eliseev, A. Ghosh, M. E. Yelisieiev, Y. M. Vysochanskii, and S. V. Kalinin, *Anomalous polarization reversal in strained thin films of $CuInP_2S_6$*, Phys. Rev. B **108**, 054107 (2023).

27. A. Ghosh*, S.V. Kalinin, and M. Ziatdinov, *Discovery of structure-property relations for molecules via hypothesis-driven active learning over the chemical space*, APL Mach. Learn. **1**, 046102 (2023).

26. S.V. Kalinin, O. Dyck, A. Ghosh, B. G. Sumpter and M. Ziatdinov, Unsupervised Machine Learning Discovery of Chemical Transformation Pathways from Atomically-Resolved Imaging Data, APL Mach. Learn. **1**, 026117 (2023).

25. D. Mukherjee, K. M. Roccapriore, A. Al-Najjar, A. Ghosh, J. D. Hinkle, A. R Lupini, R. K. Vasudevan, S. V. Kalinin, O. S. Ovchinnikova, M. A. Ziatdinov, and N. S. Rao, *A roadmap for edge computing enabled automated multidimensional transmission electron microscopy*, Microscopy Today **30**, 16 (2022).

24. S.V. Kalinin, R. Vasudevan, Y. Liu, A. Ghosh, K. Roccapriore, and M. Ziatdinov, Probe microscopy is all you need, Mach. Learn.: Sci. Technol. **4**, 023001, (2023).

23. K. M. Roccapriore, M. G. Boebinger, O. Dyck, A. Ghosh, R. Unonic, S.V. Kalinin, and M. Ziatdinov, *Probing electron beam induced transformations on a single-defect level via automated scanning transmission electron microscopy*, ACS nano **16**, 17116 (2022).

22. M. Ziatdinov, A. Ghosh, T. Wong, and S. V. Kalinin , *AtomAI: A Deep Learning Framework for Analysis of Image and Spectroscopy Data in (Scanning) Transmission Electron Microscopy and Beyond*, Nat. Mach. Intell. **4**, 1101 (2022).

21. D. Joseph, M. Shaikh, S. Buvaneswaran, T. Sahoo, A. Ghosh*, and S. Ghosh, *First-principles study of ferroelectric and optical properties in derivatives of thiourea*, J. Phys. Chem. C. **126**, 13920 (2022).

20. A. Ghosh*, G. Palanichamy, D. P. Trujillo and S. Ghosh, *Insights into cation ordering of double perovskite oxides from machine learning and causal relations*, Chem. Mater. **34**, 7563 (2022). *Featured as front cover of journal.*

19. S. V. Kalinin, A. Ghosh, R. K. Vasudevan and M. Ziatdinov, *From atomically resolved imaging to generative and causal models*, Nat. Phys. **18**, 1152 (2022).

18. A. Ghosh*, M. Ziatdinov, O. Dyck, B.G. Sumpter, and S. V. Kalinin, *Bridging microscopy with molecular dynamics and quantum simulations: An AtomAI based pipeline*, npj Comput. Mater. **8**, 74 (2022).

17. M. Ziatdinov, A. Ghosh, and S. V. Kalinin , *Physics makes the difference: Bayesian optimization and active learning via augmented Gaussian process*, Mach. Learn.: Sci. Technol. **3**, 015022 (2022).

16. R. K. Vasudevan, A. Ghosh, M. Ziatdinov and S. V. Kalinin , *Exploring Electron Beam Induced Atomic Assembly via Reinforcement Learning in a Molecular Dynamics Environment*, Nanotechnology **33**, 115301 (2021).

15. A. Ghosh, C. T. Nelson, M. Oxley, X. Zhang, M. Ziatdinov, I. Takeuchi and S. V. Kalinin, *Deep learning ferroelectric polarization distributions from STEM data via with and without atom finding*, npj Comput. Mater. **7**, 149 (2021).

14. S.V. Kalinin, M. Ziatdinov, J. Hinkle, S. Jesse, A. Ghosh, K. P. Kelley, A. R. Lupini, B. G. Sumpter and R. K Vasudevan, *Automated and Autonomous Experiment in Electron and Scanning Probe Microscopy*, ACS Nano **15**, 12604 (2021).

13. A. Ghosh, B. G. Sumpter, O. Dyck, S. V. Kalinin and M. Ziatdinov, *Ensemble learning and iterative training (ELIT) machine learning: applications towards uncertainty quantification and automated experiment in atom-resolved microscopy*, npj Comput. Mater. **7**, 100 (2021).

12. D. P. Trujillo, A. Ghosh, S. Nakhmanson, S. Sahoo and S. P. Alpay, *Surface Structure and Energetics of Low Index Facets of Bismuth Ferrite*, Phys. Chem. Chem. Phys. **22**, 16400 (2020).

11. G. Pilania, A. Ghosh, S. Hartman, C. R. Stanek and B. P. Uberuaga, *"Anion Order in Oxysulfide Perovskites: Origins and Implications"*, npj Comput. Mater. **6**, 1 (2020).

10. A. Ghosh*, F. Ronning, S. Nakhmanson and J-X Zhu, *"Machine learning study of magnetism in uranium-based compounds"*, Phys. Rev. Mater. **4**, 64414 (2020).

9. A. Ghosh*, D.P. Trujillo, H. Choi, S. M. Nakhmanson, S. P. Alpay and J.-X. Zhu, *Electronic and Magnetic Properties of Lanthanum and Strontium Doped Bismuth Ferrite: A First-Principles Study*, Sci. Rep. **9**, 194 (2019).

8. A. Ghosh, L. Louis, K. Arora, B. Hancock, J. Krzyzaniak, P. Meenan, S. Nakhmanson and G. Wood, *Assessment of Machine Learning Approaches for Predicting the Crystallization Propensity of Active Pharmaceutical Ingredients*, Cryst. Eng. Comm. **21**, 1215 (2019). *Featured as front cover of journal.*

7. G. Dhakal, M. M. Hosen, A. Ghosh, C. Lane, K. Dimitri, K. Grnicka, M. J. Winiarski, F. Kabir, C. Sims, S. Regmi, W. Neff, D. Kaczorowski, J-X. Zhu, T. Klimczuk and M. Neupane, *"Observation of topological surface state in a superconducting material"*, arXiv:1911.08519 (2019).

6. A. Ghosh, L. Louis, A. Asandei and S. M. Nakhmanson, *First-principles studies of spontaneous polarization in mixed poly (vinylidene fluoride)/2, 3, 3, 3-tetrafluoropropene polymer crystals*, Soft Matter **14**, 2484 (2018).

5. L. Louis, K. C. Pitike, A. Ghosh, S. Poddar, S. Ducharme and S. Nakhmanson, *Polarization canting in ferroelectric diisopropylammonium-halide molecular crystals: a first principles study*, J. Mater. Chem. C **6**, 1143 (2018).

4. A. Ghosh*, T. Ahmed, D. A. Yarotski, S. M. Nakhmanson and J-X. Zhu, *Oxygen vacancy effects on double perovskite Bi_2FeMnO_6: A first-principles study*, Europhys. Lett. **116**, 57002 (2017).

3. N. S. Fernando, N. T. Nunley, A. Ghosh, C. M. Nelson, J. A. Cook, A. A. Medina and S. Zollner, *Temperature dependence of the interband critical points of bulk Ge and strained Ge on Si*, Appl. Surf. Sci. **421**, 905 (2017).

2. R. Hazbun, J. Hart, R. Hickey, A. Ghosh, N. Fernando, S. Zollner, T. N. Adam and J. Kolodzey,*Silicon Epitaxy using Tetrasilane at Low Temperatures in Ultra High Vacuum Chemical Vapor Deposition*, J. Cryst. Growth **444**, 21 (2016).

1. A. Ghosh, C. M. Nelson, L. S. Abdallah and S. Zollner, *Optical constants and band structure of trigonal NiO*, J. Vac. Sci. Technol. A **33**, 061203 (2015).

INVITED PRESENTATIONS (2020 – Present)

32. **Learning materials physics from causal structures**
A. Ghosh
***2025**, Machine Learning in Chemical and Materials Sciences, Santa Fe, NM, USA*

31. **Advanced materials meet causal learning**
A. Ghosh
***2025**, ARROWS Workshop, Colorado School of Mines, CO, USA*

30. **Causal learning in advanced materials discovery**
A. Ghosh
***2025**, NASA Glenn Research Center, USA*

29. **Causal learning for advanced materials**
A. Ghosh
2025, *TMS Annual Meeting, Las Vegas, NV, USA*

28. **Synergizing Theory, Machine Learning, and Experiments in Functional Materials Dynamics**
A. Ghosh
2025, *SIAM Computational Sciences & Engineering, Dallas, TX, USA*

27. **Physics-infused causal and hypothesis-driven AI for advanced functional materials**
A. Ghosh
2024, *Materials Science & Technology, Pittsburgh, PA, USA*

26. **Causal Machine Learning Insights into Ferroics from Atomistic Simulations**
A. Ghosh
2024, *3DFeM: Center for 3D Ferroelectric Microelectronics, Pennsylvania State University, USA*

25. **Combining Predictive Machine Learning and Causal Models for Functional Materials Design**
A. Ghosh
2024, *SIAM Mathematical Aspects of Materials Science, PA, USA*

24. **Physics-informed causal and hypothesis-driven AI for advanced functional materials**
A. Ghosh
2024, *Seagate Virtual AI/ML Distinguished Speaker Series, USA*

23. **Materials design from atomistic simulations and electron microscopy guided by explainable scientific machine learning**
A. Ghosh
2024, *MRS/ACerS Joint AI and ML Virtual Workshop, USA*

22. **Artificial intelligence for physical sciences**
A. Ghosh
2024, *Invited technology talk, Oak Ridge Public Library, Oak Ridge, TN, USA*

21. **Extracting design rules for materials from atomistic simulations guided by scientific machine learning and causal relations**
A. Ghosh
2023, *Invited presentation, Dept. of Physics, Rensselaer Polytechnic Institute, NY, USA*

20. **Predictive materials design and discovery with causal machine learning**
A. Ghosh
2023, *Materials Research Society, Boston, Massachusetts, USA*

19. **Physics-informed machine learning workflows connecting electron microscope to atomistic simulations**
A. Ghosh
2023, *Materials Research Society, Boston, Massachusetts, USA*

18. **Structure-property relationships derived from electron microscope to atomistic simulations**
A. Ghosh
2023, *Materials Science & Technology, Columbus, Ohio, USA*

17. **Causality and machine learning models of ferroics from atomistic simulations**
A. Ghosh
2023, *Materials Science & Technology, Columbus, Ohio, USA*

16. **Hypothesis-Driven Active Learning for Materials**
A. Ghosh
2023, *20th International Microscopy Congress, Busan, South Korea*

15. **Structural modes in perovskite oxides derived from causal machine learning**
A. Ghosh
2023, *20th International Microscopy Congress, Busan, South Korea*

14. **Machine learning guided structural mode engineering in perovskite oxides**
A. Ghosh
2023, *Center for Nanophase Materials Sciences workshop, Knoxville, TN, USA*

13. **Structural mode engineering in perovskite oxides guided by machine learning and causal relations**
A. Ghosh
2023, *Division seminar, Computational Sciences & Engineering Division, Oak Ridge National Laboratory, TN, USA*

12. **Active and causal learning over chemical spaces for understanding structure-property relationships**
A. Ghosh
2023, *AI Initiative AISD all-hands meeting, Oak Ridge National Laboratory, TN, USA*

11. **Structural mode engineering in perovskite oxides guided by machine learning and causal relations**
A. Ghosh
2023, *Division seminar, Computational Sciences & Engineering Division, Oak Ridge National Laboratory, TN, USA*

10. **Structure-property relations in perovskite oxides using causal machine learning**
A. Ghosh
2023, *Evolution of Electronic Structure Theory and Experimental Realization, Chennai, Tamil Nadu, India*

9. **Hypothesis-driven active learning for materials**
A. Ghosh
2023, *Conference on Data Analysis (CoDA), Los Alamos National Laboratory, Santa Fe, New Mexico, USA*

8. **Causal mechanisms for learning structure-property relations in perovskite oxides**
A. Ghosh
2023, *Conference on Electronic Materials and Applications (EMA), ACerS, Orlando, Florida, USA*

7. ***Keynote lecture:*** **Causality and generative models of ferroics from high-resolution microscopy data**
A. Ghosh
2022, *Materials Congress, German Materials Society, Darmstadt, Germany*

6. **Physics-informed machine learning for electron microscopes to atomistic simulations**
A. Ghosh
2022, *Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Chennai, India*

5. **There and back again: Building workflows from electron microscope to atomistic simulations**
A. Ghosh
2022, *Department of Chemistry Colloquium, Indian Institute of Technology, Indore, India*

4. **Understanding trajectories: From electron microscopes to atomistic simulations**
A. Ghosh
2022, *Applied AI Speaker Series, Argonne National Laboratory, Illinois, USA*

3. **3Ms of My Career: Materials, Machine Learning & Michigan**
A. Ghosh
2020, *University of Michigan-Flint, MI, USA*

2. **Machine learning studies of functional materials**
A. Ghosh
2020, *Indian Institute of Technology, Bombay, India*

1. **Exploring Functional Materials with Machine Learning**
A. Ghosh
2020, *12th Asia Pacific Microscopy Conference, Hyderabad, India*

CONFERENCE PRESENTATIONS (2012 – Present)

34. **Causal Insights into Materials**
A. Ghosh
2024, *Poster presentation at Computing & Computational Sciences Directorate Advisory Board Meeting, ORNL, USA*

33. **Clarity in complexity: Solving materials science puzzles with explainable machine learning**
A. Ghosh, M. L. Pasini, J. Gounley
2024, *Poster presentation at SOS26 Conference, Cocoa Beach, FL, USA*

32. **Deriving structure-functionality relationships for materials through causal machine learning**
A. Ghosh
2023, *Poster presentation at Monterey Data Conference, Monterey, CA, USA*

31. **Deriving structure-functionality relationships for materials through causal machine learning**
A. Ghosh, Z. Fox
2023, *Poster presentation at ORNL Software Expo, Oak Ridge, TN, USA*

30. **Causal relations in determining functionalities in perovskite oxides**
A. Ghosh, S. Ghosh
2023, *American Physical Society March Meeting, Las Vegas, Nevada, USA*

29. **Hypothesis-driven active learning over the chemical space**
A. Ghosh, S. V. Kalinin, M. Ziatdinov
2023, *American Physical Society March Meeting, Las Vegas, Nevada, USA*

28. **Finding Features from Microscopes to Simulations Via Ensemble Learning and Atomic Manipulation**
A. Ghosh, B. G. Sumpter, O. Dyck, S. V. Kalinin, M. Ziatdinov
2022, *Microscopy and Microanalysis Meeting , Portland, Oregon, USA*

27. **Structural Bayesian Optimization for Active Physical Learning: Applications in Ferroelectrics and Magnetic Systems**
A. Ghosh, S. V. Kalinin, M. Ziatdinov
2022, *American Physical Society March Meeting, Chicago, Illinois, USA*

26. **Deep Learning framework towards automated experiments and quantum simulations**
A. Ghosh, B. G. Sumpter, O. Dyck, S. V. Kalinin, M. Ziatdinov
2022, *American Physical Society March Meeting, Chicago, Illinois, USA*

25. **AtomAI for deep learning for microscopic images**
A. Ghosh, S. V. Kalinin, M. Ziatdinov
2022, *Electronic Materials and Applications, Orlando, Florida, USA*

24. **Mapping Polarization from STEM and STM Images**
A. Ghosh, C. T. Nelson, M. Oxley, X. Zhang, M. Ziatdinov, I. Takeuchi, S. V. Kalinin
2022, *Materials Research Society Fall Meeting, Boston, MA, USA*

23. **Supervised machine learning of imaging data: DCNNs go ELIT**
Tutorial Presenter: A. Ghosh, M. Ziatdinov
2021, *Virtual School - Machine Learning and Automated Experiment in Scanning Probe Microscopy, ORNL, TN, USA*

22. **Connecting Pathways of Microscopic Images and First-principles simulations via deep learning**
A. Ghosh, S. V. Kalinin, M. Ziatdinov
2021, *Materials Research Society Fall Meeting, Boston, MA, USA*

21. **Incorporating Physical Priors Into probabilistic models in Bayesian framework**
A. Ghosh, S. V. Kalinin, M. Ziatdinov
2021, *Materials Research Society Fall Meeting, Boston, MA, USA*

20. **Machine Learning on Experimental Data for Emergent Quantum Materials**
A. Ghosh, S. V. Kalinin, M. Ziatdinov
2021, *Materials Research Society Fall Meeting, Boston, MA, USA*

19. **Direct mapping of polarization fields from STEM images: A Deep Learning based exploration of ferroelectrics**
A. Ghosh, C. T. Nelson, M. Oxley, X. Zhang, M. Ziatdinov, I. Takeuchi, S. V. Kalinin
2021, *Materials Research Society Fall Meeting, Boston, MA, USA*

18. **AtomAI: Microscopic Images to Atomistic Simulations to Learning and Discovering Physics**
A. Ghosh, S. V. Kalinin, M. Ziatdinov
2021, *ORNL Software Data Expo, Oak Ridge, TN, USA*

17. **Fusing physical laws and probability in active learning in a Bayesian setting**
A. Ghosh, S. V. Kalinin, M. Ziatdinov
***2021**, CIFAR Deep Learning Summer School, Canada*

16. **Data-driven study of magnetic interactions of transition-metal based 2D materials**
A. Ghosh, S. Lin, J.-X. Zhu
***2020**, American Physical Society March Meeting, Denver, CO, USA*

15. **Exploring Organic Ferroelectrics Using Data-driven Approaches**
A. Ghosh, N. Lubbers, S. Nakhmanson, J.-X. Zhu
***2020**, American Physical Society March Meeting, Denver, CO, USA*

14. **A Machine Learning Study of Magnetism in Actinides**
A. Ghosh, F. Ronning, S. M. Nakhmamson, J.-X. Zhu
***2020**, Electronic Materials and Applications conference, Orlando, FL, USA*

13. **Design of novel molecular ferroelectrics using first-principles based and machine learning approaches**
A. Ghosh, L. Louis, K. C. Pitike, S. Poddar, S. Ducharme, A. D. Asandei, N. Lubbers, S. Nakhmanson
***2020**, Electronic Materials and Applications conference, Orlando, FL, USA*

12. **Understanding Magnetic Properties of Uranium-Based Binary Compounds from Machine Learning**
A. Ghosh, F. Ronning, S. M. Nakhmamson, J.-X. Zhu
***2019**, American Physical Society March Meeting, Boston, MA, USA*

11. **Predicting Crystallization Propensity using Machine Learning Approaches**
A. Ghosh, L. Louis, K. Arora, B. Hancock, J. Krzyzaniak, P. Meenan, S. Nakhmanson and G. Wood
***2019**, Computational Data Science Approaches for Materials Conference, Los Alamos, NM, USA*

10. **Machine Learning in Understanding Magnetic Properties of Uranium-Based Binary Compounds**
A. Ghosh, F. Ronning, S. M. Nakhmanson, J.-X. Zhu
***2018**, Seminar at Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM, USA*

9. **First-principles based design of novel organic ferroelectrics: The cases of PVDF and DIPA materials templates**
A. Ghosh, L. Louis, K. C. Pitike, S. Poddar, S. Ducharme, A. D. Asandei, S. M. Nakhmanson
***2018**, XXIII Czech-Polish Seminar, Kouty, Czech Republic*

8. **Exploring dopants and vacancy effects in $Bi_{1-x}M_xFeO_3$(M=La,Sr) and Bi_2FeMnO_6 bulk systems: A First-Principles Based Study**
A. Ghosh, H. Choi, D. P. Trujillo, S. M. Nakhmanson, S. P. Alpay, J.-X. Zhu
***2018**, International Conference On Current Trends In Materials Science And Engineering, Kolkata, India*

7. **Ab Initio Studies of Polar Properties of Tetrafluoropropene/Vinylidene Fluoride Copolymers**
A. Ghosh, L. Louis, A. Asandei, S. M. Nakhmanson
***2016**, Materials Research Society Fall Meeting, Boston, MA, USA*

6. **Predicting Crystallization Propensity Using Machine Learning Approaches**
A. Ghosh, L. Louis, S.M. Nakhmanson, K. Arora, B. C. Hancock, J. Krzyzaniak, P. Meenan, G.P. Wood
***2016**, Materials Research Society Fall Meeting, Boston, MA, USA*

5. **Optical Constants and Band Structure of NiO**
A. Ghosh, S. Zollner
***2015**, Annual Meeting of American Physical Society Four Corners Section, Tempe, AZ, USA*

4. **Exploring Supersonic Gas Jets using Mach-Zehnder and Nomarski Interferometry**
A. Ghosh, B. Makovicka
***2015**, Michigan Section of AAPT Spring Meeting, East Lansing, MI, USA*

3. **Strain Measurements of Ge Epilayers on Si by Spectroscopic Ellipsometry**,
Dielectric Function of NiO and Si from 25 meV to 6 eV: What's the Difference
A.Ghosh, S. Zollner
***2014**, American Physical Society March Meeting, Denver, CO, USA*

2. **Investigation of Dynamic Strains of Ge films on Si using Spectroscopic Ellipsometry**
   A. Ghosh, S. Zollner
   ***2012**, Conference for Undergraduate Women in Physical Sciences, Lincoln, NE, USA*

1. **Radiations from Blackholes may hint at the Existence of Extra Dimensions**
   A. Ghosh, J. Alsup
   ***2012**, Conference for Undergraduate Women in Physical Sciences, Lincoln, NE, USA*

WORKSHOP PARTICIPATIONS (2016 – Present)

11. **(*Invited presenter on Causality:*) AI Summer Institute**
    ***2024**, Oak Ridge National Laboratory*

10. **(*Invited presenter on Introduction to Machine Learning:*) Next Generation Pathways Summer School, Oak Ridge National Laboratory, USA**
    ***2024**, Oak Ridge National Laboratory*

9. **(*Tutorial presenter:*) Summer school on Machine Learning in Electron Microscopy**
   ***2023**, Virtual*

8. **(*Tutorial presenter:*) International school and conference on Evolution of Electronic Structure Theory and Experimental Realization**
   ***2023**, Virtual*

7. **(*Scribe:*) AI for Science and Security Workshop**
   ***2022**, Tennessee State University, Nashville, TN*

6. **(*Tutorial presenter:*) Virtual School - Machine Learning and Automated Experiment in Scanning Probe Microscopy**
   ***2021**, Oak Ridge National Laboratory, Oak Ridge, TN*

5. **(*Poster presenter:*) CIFAR Deep Learning Summer School**
   ***2021**, Virtual*

4. **(*Tutorial presenter:*) AI for Atoms: How to Machine Learn STEM Workshop**
   ***2020**, Oak Ridge National Laboratory, Oak Ridge, TN*

3. **LAMMPS Workshop**
   ***2019**, University of New Mexico, Albuquerque, NM*

2. **NOMAD Summer: A Hands-on Course on Tools for Novel-Materials Discovery**
   ***2017**, Humboldt University of Berlin , Germany*

1. **(*Poster presenter:*) NSF-CECAM School on Computational Materials Science**
   ***2017**, CECAM, EPFL, Lausanne, Switzerland*

SKILLS

- **Computational methods**: Density Functional Theory (DFT), Pseudopotential-plane wave based techniques, LAPW, DFTB, molecular dynamics (MD), *ab initio* MD (AIMD), band structure techniques, atomic orbital techniques for organic molecules
- **Programming languages and frameworks for ML/AI**: Python, R, PyTorch, TensorFlow, Scikit-Learn
- **Advanced computational software for materials modeling**: VASP, Quantum Espresso, Gaussian, LAMMPS, MOOSE, FERRET, RAVEN
- **Technical tools for research and presentation**: LaTeX, Mathematica, WVASE, Matlab, Paraview, Labview, Vesta, MS Office, HTML
- **Miscellaneous**: Qiskit Learn, SQLite, SQL