

Yongtao LIU

Center for Nanophase Materials Science

Oak Ridge National Laboratory, Oak Ridge, TN, USA

Email: liuy3@ornl.gov

[Google Scholar](#); [LinkedIn](#)

Highlights

- Lead/Corresponding author on 35+ publications, and co-authored 70+ publications.
- Delivered 10+ invited talks, and presented 40+ contributed and poster presentations at prestigious conferences.
- Honored with 10+ research awards, including the R&D 100 Award and the Microscopy Today Innovation Award, etc.
- Actively engaged in research communities: organized 5+ symposia and workshops in past two years.

EDUCATION

The University of Tennessee, Knoxville, Tennessee, United States 2016.08—2020.12

- Ph.D., Materials Science and Engineering

Nankai University, Tianjin, China 2010.09—2014.08

- BS, College of Chemistry

WORK AND RESEARCH HISTORY

R&D Staff 10.2024—present

Data NanoAnalytics Group, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee, United States

- Leading an INTERSECT project for cross-facility co-optimization combining AI-driven autonomous synthesis platform and autonomous characterization platform

R&D Associate Staff 04.2023—09.2024

Data NanoAnalytics Group, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee, United States

- Focused on automated and autonomous experiment harnessing the power of machine learning for physics and materials discovery.
- Developing platform for automated microscopy, *i.e.*, *AEcroscopy*
- Spearheaded the project of *Gated Active Learning for Reliable Autonomous Experiment*

Postdoctoral Research Associate 04.2021—03.2023

Functional Atomic Force Microscopy Group, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee, United States

- Investigating novel ferroelectric materials using scanning probe microscopy

Graduate Research Assistant 08.2016—12.2020

Department of Materials Science and Engineering, The University of Tennessee, Knoxville, Tennessee, United States

- Exploring fundamental mechanisms of metal halide perovskite with functional and chemical imaging techniques, including synthesizing metal halide perovskite thin films.

HONORS AND AWARDS

- **Microscopy Today Innovation Awards**, Microscopy Society of America, 2024
- **AVS NSTD Early Career Competition Finalist**, American Vacuum Society, 2023
- **R&D 100 Award**, 2023
- **Center for Nanophase Materials Sciences (CNMS) Postdoctoral Award**, 2023
- **Microscopy & Microanalysis Postdoctoral Scholar Award**, Microscopy Society of America, 2023
- **ORNL Outstanding Scholarly Output Award**, Oak Ridge National Laboratory, 2022
- **AVS NSTD Early Career Competition Finalist**, American Vacuum Society, 2022
- **MRS Graduate Student Silver Award**, Material Research Society (MRS), December 2019
- **AVS Graduate Research Award**, American Vacuum Society (AVS), October 2019
- **Best Student Poster Gold Award (rank 1st)**, Center for Nanophase Materials Sciences (CNMS) at Oak Ridge National Laboratory (ORNL), August 2019
- **Joseph E. Spruiell Award for Excellence in Research**, Department of Materials Science and Engineering, the University of Tennessee at Knoxville, April 2019
- **MRS Graduate Student Silver Award**, Material Research Society (MRS), November 2018
- **Best Student Poster Award**, Center for Nanophase Materials Sciences (CNMS) at Oak Ridge National Laboratory (ORNL), August 2018

FUNDING

- FY2025 ORNL DRD INTERSECT INITIATIVE
 - “Physics-Informed, Data-Fusion Approach for Cross-Facility Optimization”; Role: PI; Awarded: 360 K/ year.
 - “AI-Driven Energy Materials Synthesis and Topochemical Investigation”; Role: Co-I; Awarded: 370 K/ year.

PROFESSIONAL SERVICE

Society Committee Member

- 2024-2025: Executive Committee Member of American Vacuum Society Nanoscale Science and Technology Division
- 2025: Program Committee of the Computer Vision for Materials Science (CV4MS), Computer Vision and Pattern Recognition (CVPR)

Conference Symposium and Workshop Organizer

- (upcoming) 2025 MS&T: Materials Science & Technology: *Enhancing the Accessibility of Machine Learning-Enabled Experiments*; Sep 28 - Oct 1, 2025; Columbus, OH
- (upcoming) 2025 ACerS EMA Basic Science and Electronic Materials Meeting: *AI in materials research: from data analysis, autonomous experimentation, to human-AI cooperation*; Feb 25-28, 2025; Denver, CO
- (upcoming) 2024 MRS Fall Meeting: *Symposium MT02-Machine Learning in Action—Automated and Autonomous Experiments*; Dec 1- 6, 2024; Boston, MA

- 2024 CNMS User Meeting: *Workshop-AI/ML approaches to incorporate theory-in-the-loop to achieve autonomous synthesis and manipulation*, August 12-15, 2024; Knoxville, TN
- 2024 Microscopy & Microanalysis Meeting: *Symposium C02-Machine Learning-driven Automated Microscopy for Materials Discovery and Semiconductor Manufacturing*; July 28-Aug 1, 2024; Cleveland, OH
- 2024 MRS/ACerS Joint Workshop: *AI/ML for Ceramics/Glasses*; Mar 26-27, 2024; Virtual
- 2024 ACerS EMA Basic Science and Electronic Materials Meeting: *Symposium S09-Machine Learning and Automated Synthesis/Characterization for Novel Materials*; Feb 13-16, 2024; Denver, CO
- 2023 MRS Fall Meeting: *Symposium DS02-Automated Experimentation with Synchrotrons, Neutrons and Microscopes*; Nov 26-Dec 1, 2023; Boston, MA
- 2023 CNMS User Meeting Workshop: *Autonomous Characterization and Synthesis*; Aug 7, 2023; Knoxville, TN

Funding Reviewer

- DOE ASCR
- ORNL INITIATIVES

Editorial Service

- 2021 – 2023: Editorial Board Member for Energy Frontier Research Centers (supported by The Department of Energy's Office of Science) Newsletter

PUBLICATIONS

Google Scholar

1. Biswas, A.*, Vasudevan, R., Pant, R., Takeuchi, I., Funakubo, H., **Liu, Y.***, SANE: Strategic Autonomous Non-Smooth Exploration for Multiple Optima Discovery in Multi-modal and Non-differentiable Black-box Functions. arXiv preprint arXiv:2409.12295 (2024).
2. Um, M., Sanchez, S. L., Song, H., Lawrie, B. J., Ahn, H., Kalinin, S. V., **Liu, Y.***, Choi, H.*, Yang, J.*, Ahmadi, M*, Tailoring Molecular Space to Navigate Phase Complexity in Cs-based Quasi-2D Perovskites via Gated-Gaussian-Driven High-Throughput Discovery, 10.26434/chemrxiv-2024-8qtk2, (2024).
3. Pratiush, U., Funakubo, H., Vasudevan, R., Kalinin, S. V.*, **Liu, Y.***, *Scientific Exploration with Expert Knowledge (SEEK) in Autonomous Scanning Probe Microscopy with Active Learning*. arXiv preprint arXiv:2408.02071, (2024).
4. Harris, S.B, Vasudevan, R.V., Ziatdinov, M.A., **Liu, Y.***, *Active oversight and quality control in standard Bayesian optimization for autonomous experiments*. arXiv preprint arXiv:2405.16230 (2024).
5. Mani, V., **Liu, Y.**, and Kalinin, S.V., *Physics and Chemistry from Parsimonious Representations: Image Analysis via Invariant Variational Autoencoders*. npj Computational Materials 10 (1), 183 (2024).
6. **Liu, Y.***, Huey, B. D., Ziatdinov, M. A., & Kalinin, S. V.* *Physical discovery in representation learning via conditioning on prior knowledge*. Journal of Applied Physics, 136(6), (2024).

7. Raghavan, A., Pratiush, U., Valletti, M., Liu, R., Emery, R., Funakubo, H., **Liu, Y.**, Rack, P., Kalinin, S., Invariant Discovery of Features Across Multiple Length Scales: Applications in Microscopy and Autonomous Materials Characterization. arXiv preprint arXiv:2408.00229, (2024).
8. Yang, J., Ievlev, A.V., Morozovska, A.N., Eliseev, E., Poplawsky, J.D., Goodling, D., Spurling, R.J., Maria, J.P., Kalinin, S.V.* and **Liu, Y.***, *Coexistence and interplay of two ferroelectric mechanisms in Zn_{1-x}MgxO*. Advanced Materials: 2404925., (2024).
9. Raghavan, A., Takeuchi, I., Eliseev, E. A., Morozovska, A.N.*, Ziatdinov, M., Kalinin, S.V.*, and **Liu, Y.***, *Evolution of ferroelectric properties in SmxBi_{1-x}FeO₃ via automated Piezoresponse Force Microscopy across combinatorial spread libraries*, ACS Nano, 2024
10. Sanchez, S. L., Foadian, E., Ziatdinov, M., Yang, J., Kalinin, S. V., **Liu, Y.***, & Ahmadi, M.* *Physics-driven discovery and bandgap engineering of hybrid perovskites*. Digital Discovery (2024).
11. Slautin, B.N., **Liu, Y.**, Funakubo, H., Vasudevan, R.K., Ziatdinov, M.A. and Kalinin, S.V., *Bayesian Co-navigation: Dynamic Designing of the Materials Digital Twins via Active Learning*. ACS Nano, (2024).
12. Biswas, A., **Liu, Y.**, Creange, N., Liu, Y.C., Jesse, S., Yang, J.C., Kalinin, S.V., Ziatdinov, M.A. and Vasudevan, R.K., *A dynamic Bayesian optimized active recommender system for curiosity-driven partially Human-in-the-loop automated experiments*. npj Computational Materials, 10(1), p.29 (2024).
13. Slautin, B.N., Pratiush, U., Ivanov, I.N., **Liu, Y.**, Pant, R., Zhang, X., Takeuchi, I., Ziatdinov, M.A. and Kalinin, S.V., *Multimodal Co-orchestration for Exploring Structure-Property Relationships in Combinatorial Libraries via Multi-Task Bayesian Optimization*. arXiv preprint arXiv:2402.02198 (2024).
14. Morozovska, A. N., Eliseev, E. A., **Liu, Y.**, Kelley, K. P., Ghosh, A., Liu, Y., ... & Kalinin, S. V. *Bending-induced isostructural transitions in ultrathin layers of van der Waals ferrielectrics*. Acta Materialia 263 (2024): 119519.
15. Slautin, B.N., **Liu, Y.**, Funakubo, H. and Kalinin, S.V., *Unraveling the Impact of Initial Choices and In-Loop Interventions on Learning Dynamics in Autonomous Scanning Probe Microscopy*. Journal of Applied Physics 135.15 (2024).
16. **Liu, Y.***, Checa, M. and Vasudevan, R.K., *Synergizing Human Expertise and AI Efficiency with Language Model for Microscopy Operation and Automated Experiment Design*. Machine Learning: Science and Technology (2024).
17. Kalinin, S. V., **Liu, Y.**, Biswas, A., Duscher, G., Pratiush, U., Roccapiore, K., ... & Vasudevan, R. *Human-in-the-loop: The future of Machine Learning in Automated Electron Microscopy*. Microscopy Today 32.1 (2024): 35-41.
18. Morozovska, A.N., Eliseev, E.A., **Liu, Y.**, Kelley, K.P., Ghosh, A., Liu, Y., Yao, J., Morozovsky, N.V., Kholkin, A.L., Vysochanskii, Y.M. and Kalinin, S.V. *Bending-induced isostructural transitions in ultrathin layers of van der Waals ferrielectrics*. Acta Materialia, 263, p.119519 (2024).
19. **Liu, Y.***, Roccapiore, K., Checa, M., Valletti, S. M., Yang, J. C., Jesse, S., & Vasudevan, R. K.*. *AEcroscoPy: A software-hardware framework empowering microscopy toward automated and autonomous experimentation*. Small Methods (2024): 2301740.

20. Kalinin, S.V., Ziatdinov, M., Ahmadi, M., Ghosh, A., Roccapiore, K., **Liu, Y.**, and Vasudevan, R.K., *Designing Workflows for Materials Characterization*. Applied Physics Reviews 11.1 (2024).
21. Ziatdinov, M. A., Yaman, M. Y., **Liu, Y.**, Ginger, D., Kalinin, S. V., *Semi-supervised learning of images with strong rotational disorder: assembling nanoparticle libraries*, Digital Discovery 3.6 (2024): 1213-1220.
22. Morozovska, A.N., Eliseev, E.A., Yurchenko, L.P., Laguta, V.V., **Liu, Y.**, Kalinin, S.V., Kholkin, A.L. and Vysochanskii, Y.M. *The strain-induced transitions of the piezoelectric, pyroelectric, and electrocaloric properties of the CuInP2S6 films*. AIP Advances, 13(12) (2023).
23. **Liu, Y.***, Ievlev, A., Casamento, J., Hayden, J., Trolrier-McKinstry, S., Maria, J. P., ... & Kelley, K. P.* *The interplay between ferroelectricity and electrochemical reactivity on the surface of binary ferroelectric AlxB1-xN*. Advanced Electronic Materials, p.2300489 (2023).
24. **Liu, Y.***, Morozovska, A. N., Ghosh, A., Kelley, K. P., Eliseev, E. A., Yao, J., ... & Kalinin, S. V.* *Stress and curvature effects in layered 2D ferroelectric CuInP2S6*. ACS Nano, (2023).
25. Jacques, L., Shetty, S., Vega, F.J., **Liu, Y.**, Aronson, B., Beechem, T. and Trolrier-McKinstry, S., *Deposition and dielectric characterization of highly oriented V2O5 thin films*. MRS communications, pp.1-6, (2023).
26. **Liu, Y.***, Ziatdinov, M., Vasudevan, R., and Kalinin, S.V.*, *Explainability and human intervention in autonomous scanning probe microscopy*. Patterns (2023).
27. Yao, J., **Liu, Y.**, Ding, S., Zhu, Y., Mao, Z., Kalinin, S. V., & Liu, Y. *Ferroelectric Schottky diodes of CuInP2S6 nanosheet*. Applied Physics Letters, 123(14), (2023).
28. Morozovska, A. N., Eliseev, E. A., Yurchenko, L. P., Laguta, V. V., **Liu, Y.**, Kalinin, S. V., ... & Vysochanskii, Y. M. *The strain-induced transitions of the piezoelectric, pyroelectric and electrocaloric properties of the CuInP2S6 films*. AIP Advances 13.12 (2023).
29. Yang, J., LaFollette, D. K., Lawrie, B. J., Ievlev, A. V., **Liu, Y.**, Kelley, K. P., ... & Ahmadi, M. *Understanding the Role of Cesium on Chemical Complexity in Methylammonium-Free Metal Halide Perovskites*. Advanced Energy Materials, 13(33), 2202880, (2023).
30. Kelley, K. P., Morozovska, A. N., Eliseev, E. A., **Liu, Y.**, Fields, S. S., Jaszewski, S. T., ... & Kalinin, S. V. *Ferroelectricity in hafnia controlled via surface electrochemical state*. Nature Materials, 1-8, (2023).
31. Hysmith, H., Park, S. Y., Yang, J., Ievlev, A. V., **Liu, Y.**, Zhu, K., ... & Ovchinnikova, O. S. *The Role of SnO2 Processing on Ionic Distribution in Double-Cation–Double Halide Perovskites*. ACS Applied Materials & Interfaces, 15(30), 36856-36865, (2023).
32. Kalinin, S. V., Dyck, O., Ghosh, A., **Liu, Y.**, Proksch, R., Sumpter, B. G., Ziatdinov, M., *Unsupervised machine learning discovery of structural units and transformation pathways from imaging data*. APL Machine Learning, 1(2), (2023).
33. Kalinin, S.V., Vasudevan, R.K., **Liu, Y.**, Ghosh, A., Roccapiore, K., and Ziatdinov, M., *Probe Microscopy is All You Need*. Machine Learning: Science and Technology 4, 4, (2022).
34. **Liu, Y.***, Yang, J., Vasudevan, R.K., Kelley, K.P., Ziatdinov, M., Kalinin, S.V.*, and Ahmadi, M.* *Exploring the Relationship of Microstructure and Conductivity in Metal Halide Perovskites via Active Learning-Driven Automated Scanning Probe Microscopy*. The Journal of Physical Chemistry Letters 14.13 (2023): 3352-3359.

35. Sanchez, S., **Liu, Y.**, Yang, J., Kalinin, S. V., Ziatdinov, M., & Ahmadi, M. *Exploring the Evolution of Metal Halide Perovskites via Latent Representations of the Photoluminescent Spectra*. Advanced Intelligent Systems, 5(5), 2200340, (2023).
36. **Liu, Y.***, Yang, J., Lawrie, B.J., Kelley, K.P., Ziatdinov, M., Kalinin, S.V. *, and Ahmadi, M.* *Disentangling electronic transport and hysteresis at individual grain boundaries in hybrid perovskites via automated scanning probe microscopy*. ACS nano, 17, 10, 9647–9657 (2023).
37. **Liu, Y.***, Morozovska, A.N., Eliseev, E.A., Kelley, K.P., Vasudevan, R., Ziatdinov, M. *, Kalinin, S.V. *, *Autonomous scanning probe microscopy with hypothesis learning: Exploring the physics of domain switching in ferroelectric materials*. Patterns 4.3 (2023).
38. **Liu, Y.**, Vasudevan, R.K., Kelley, K.P., Funakubo, H., Ziatdinov, M., and Kalinin, S.V., *Learning the right channel in multimodal imaging: automated experiment in Piezoresponse Force Microscopy*. npj Computational Materials, 9(1), 34. (2022).
39. **Liu, Y.**, Kelley, K.P., Vasudevan, R.K., Zhu, W., Hayden, J., Maria, J-P., Funakubo, H., Ziatdinov, M., Trolier-McKinstry, S., and Kalinin, S.V., *Automated Experiments of Local Non-linear Behavior in Ferroelectric Materials*. Small, 202204130 (2022).
40. **Liu, Y.**, Kelley, K.P., Funakubo, H., Kalinin, S.V., and Ziatdinov, M., *Exploring Physics of Ferroelectric Domain Walls in Real Time: Deep Learning Enabled Scanning Probe Microscopy*. Advanced Science, 2203957 (2022)
41. Maxim, Z., **Liu, Y.**, Kelley, K., Vasudevan, R., and Kalinin, S.V., *Bayesian Active Learning for Scanning Probe Microscopy: from Gaussian Processes to Hypothesis Learning*. ACS Nano, 16, 9, (2022).
42. Maxim, Z., **Liu, Y.**, and Kalinin, S.V., *Active learning in open experimental environments: selecting the right information channel (s) based on predictability in deep kernel learning*. arXiv preprint arXiv:2203.10181 (2022).
43. Ziatdinov, M., **Liu, Y.**, Morozovska, A.N., Eliseev, E.A., Zhang, X., Takeuchi, I., Kalinin, S.V., *Hypothesis learning in an automated experiment: application to combinatorial materials libraries*. Advanced Materials, 202201345 (2021).
44. Kim, D., Lim, J., Lee, S., Soufiani, A.M., Choi, F., Ievlev, A.V., Borodinov, N., **Liu, Y.**, Ovchinnikova, O.S., Ahmadi, M., Lim, S., Sharma, P., Seidel, J., Noh, J.H., Yun, J.S., *Microstructural Evaluation of Phase Instability in Large Bandgap Metal Halide Perovskites*. ACS nano 15, no. 12 (2021): 20391-20402.
45. **Liu, Y.**, Fields, S.S., Mimura, T., Kelley, K.P., Ihlefeld, J.F., Kalinin, S.V., *Exploring leakage in dielectric films via automated experiment in scanning probe microscopy*. Applied Physics Letter, 120, 182903 (2022).
46. Kalinin, S.V., Steffes, J.J., **Liu, Y.**, Huey, B.D., Ziatdinov, M., *Disentangling ferroelectric domain wall geometries and pathways in dynamic piezoresponse force microscopy via unsupervised machine learning*. Nanotechnology 33, no. 5 (2021): 055707.
47. Kim, D., **Liu, Y.**, Ievlev, A.V., Higgins, K., Ovchinnikova, O.S., Yun, J.S., Seidel, J., Kalinin, S.V., and Ahmadi, M., *Unraveling the hysteretic behavior at double cations-double halides perovskite-electrode interfaces*. Nano Energy 89 (2021): 106428.
48. **Liu, Y.**, Vasudevan, R.K., Kelley, K.P., Kim, D., Sharma, Y., Ahmadi, M., Kalinin, S.V., and Ziatdinov, M., *Decoding the shift-invariant data: applications for band-excitation scanning probe microscopy*. Machine Learning: Science and Technology 2, no. 4 (2021): 045028.

49. **Liu, Y.**, Ziatdinov, M., Kalinin, S. V., *Exploring causal physical mechanisms via non-gaussian linear models and deep kernel learning: applications for ferroelectric domain structures*. ACS Nano 2022 16 (1), 1250-1259, DOI: 10.1021/acsnano.1c09059
50. **Liu, Y.**, Kelley, K. P., Vasudevan, R. K., Funakubo, H., Ziatdinov, M. A., Kalinin, S. V., *Experimental discovery of structure-property relationships in ferroelectric materials via active learning*, Nature Machine Intelligence, 4, 341-350, (2022), DOI:10.1038/s42256-022-00460-0.
51. **Liu, Y.**, Wang, M., Ievlev, A. V., Ahmadi, M., Hu, B., Ovchinnikova, O. S., *Photoinduced iodine expulsion and halides-demixing in metal halide perovskites*, Materials Today Nano (2022): 100197.
52. **Liu, Y.***, Proksch, R., Wong, C. Y., Ziatdinov, M., Kalinin, S. V., *Disentangling ferroelectric wall dynamics and identification of pinning mechanisms via deep learning*, Advanced Materials, 202103680 (2021).
53. **Liu, Y.**, Kim, D., Ievlev, A. V., Kalinin, S. V., Ahmadi, M., Ovchinnikova, O. S., *Ferroic halide perovskite optoelectronics*, Advanced Functional Materials, 202102793 (2021).
54. bin Mohd Yusoff, A. R., Mahata, A., Vasilopoulou, M., Ullah, H., Hu, B., da Silva, W. J., Schneider, F. K., Gao, P., Ievlev, A. V., **Liu, Y.**, Ovchinnikova, O. S., Angelis, F. D., Nazeeruddin, M. K., *Observation of large Rashba spin-orbit coupling at room temperature in compositionally engineered perovskite single crystals and application in high performance photodetectors*. Materials Today (2021), doi: 10.1016/j.mattod.2021.01.027.
55. **Liu, Y.**, Borodinov, N., Collins, L., Ovchinnikova, O. S., Ievlev, A. V., *Role of Decomposition Product Ions in Hysteretic Behavior of Metal Halide Perovskite*. ACS nano (2021), doi: 10.1021/acsnano.1c02097.
56. **Liu, Y.**, Trimby, P., Collins, L., Ahmadi, M., Winkelmann, A., Proksch, R., Ovchinnikova, O. S., *Correlating crystallographic orientation and ferroic behavior of twin domains in metal halide perovskite*, ACS nano 15 (4): 7139-7148, (2021).
57. **Liu, Y.**, Sumpter, B. G., Keum, J. K., Hu, B., Ahmadi, M., Ovchinnikova, O. S., *Strain in Metal Halide Perovskites: The Critical Role of A-Site Cation*. ACS Applied Energy Materials 4 (3): 2068-2072, (2021).
58. **Liu, Y.**, Ievlev, A. V., Collins, L., Borodinov, N., Belianinov, A., Lorenz, M., Jesse, S., Xiao, K., Ahmadi, M., Hu, B., Kalinin, S. V., Ovchinnikova, O. S., *Direct observation of photoinduced ion migration in lead halide perovskites*, Advanced Functional Materials, 2008777 (2020).
59. **Liu, Y.**, Borodinov, N., Lorenz, M., Ahmadi, M., Kalinin, S. V., Ievlev, A. V., Ovchinnikova, O. S., *Hysteretic Ion Migration and Remanent Field in Metal Halide Perovskites*, Advanced Science, 2001176 (2020).
60. **Liu, Y.**, Lorenz, M., Ievlev, A. V., Ovchinnikova, O. S., *Secondary Ion Mass Spectrometry (SIMS) for chemical characterization of metal halide perovskites*, Advanced Functional Materials, 2002201 (2020).
61. Dou, Y., Xu, H., **Liu, Y.**, Wang, M., Zhang, J., Ovchinnikova, O. S., Hu, B. *Tuning spin-orbit coupling towards enhancing photocurrent in hybrid organic-inorganic perovskites by using mixed organic cations*. Organic Electronics, 105671 (2020).
62. **Liu, Y.**, Ievlev, I.V., Collins, C., Belianinov, A., Keum, J.K., Ahmadi, M., Jesse, S., Retterer, S.T., Xiao, K., Huang, J., Sumpter, B.G., Kalinin, S.V., Hu, B., Ovchinnikova, O.S., *Strain-*

Chemical Gradient and Polarization in Metal Halide Perovskites. Advanced Electronic Materials, 1901235 (2020).

63. **Liu, Y.**, Li, M., Wang, M., Collins, L., Ievlev, A.V., Jesse, S., Xiao, K., Hu, B., Belianinov, A., Ovchinnikova, O.S., *Twin domains modulate light-matter interactions in metal halide perovskites*, APL Materials, 8(1), p.011106 (2020).
64. Zhu, X., Xu, H., **Liu, Y.**, Zhang, J., Wang, M., Ivanov, I.N., Ovchinnikova, O.S., Hu, B., *Two-Photon Up-Conversion Photoluminescence Realized through Spatially Extended Gap States in Quasi-2D Perovskite Films*. Advanced Materials, 1901240 (2019).
65. **Liu, Y.**, Belianinov, A., Collins, L., Proksch, R., Ievlev, A.V., Hu, B., Kalinin, S.V., Ovchinnikova, O.S., *Ferroic twin domains in metal halide perovskites*, MRS Advances, 4(51-52), p.2817, (2019).
66. **Liu, Y.**, Ievlev, A.V., Borodinov, N., Collins, L., Belianinov, A., Keum, J.K., Ahmadi, M., Jesse, S., Xiao, K., Huang, J., Sumpter, B.G., Hu, B., Kalinin, S.V., and Ovchinnikova, O.S., *Light-ferroic interaction in hybrid organic inorganic perovskites*, Advanced Optical Materials, 1901451 (2019).
67. **Liu, Y.**, Collins, L., Proksch, R., Kim, S., Watson, B.R., Doughty, B., Calhoun, T.R., Ahmadi, M., Ievlev, A.V., Jesse, S., Retterer, S.T., Belianinov, A., Xiao, K., Huang, J., Sumpter, B.G., Kalinin, S.V., Hu, B., and Ovchinnikova, O.S., *Reply to: On the ferroelectricity of $\text{CH}_3\text{NH}_3\text{PbI}_3$ perovskites*. Nature materials, 18(10), p.1051, (2019).
68. Collins, L., **Liu, Y.**, Ovchinnikova, O.S., & Proksch, R., *Quantitative Electromechanical Atomic Force Microscopy*. ACS Nano, 13(7), p.8055, (2019).
69. **Liu, Y.**, Collins, L., Proksch, R., Kim, S., Watson, B.R., Doughty, B., Calhoun, T.R., Ahmadi, M., Ievlev, A.V., Jesse, S., Retterer, S.T., Belianinov, A., Xiao, K., Huang, J., Sumpter, B.G., Kalinin, S.V., Hu, B., and Ovchinnikova, O.S., *Chemical nature of ferroelastic twin domains in $\text{CH}_3\text{NH}_3\text{PbI}_3$ perovskite*. Nature materials, 17(11), p.1013, (2018).
70. **Liu, Y.**, Collins, L., Belianinov, A., Neumayer, S.M., Ievlev, A.V., Ahmadi, M., Xiao, K., Retterer, S.T., Jesse, S., Kalinin, S.V., Hu, B., and Ovchinnikova, O.S., *Dynamic behavior of $\text{CH}_3\text{NH}_3\text{PbI}_3$ perovskite twin domains*. Applied Physics Letters, 113(7), p.072102, (2018).
71. Collins, L., Ahmadi, M., Qin, J., **Liu, Y.**, Ovchinnikova, O.S., Hu, B., Jesse, S. and Kalinin, S.V., *Time resolved surface photovoltage measurements using a big data capture approach to KPFM*. Nanotechnology, 29(44), p.445703, (2018).
72. **Liu, Y.**, Sun, Y., Li, M., Feng, H., Ni, W., Zhang, H., Wan, X. and Chen, Y., *Efficient carbazole-based small-molecule organic solar cells with an improved fill factor*. RSC Advances, 8(9), p.4867, (2018).
73. Zhang, H., **Liu, Y.**, Sun, Y., Li, M., Ni, W., Zhang, Q., Wan, X. and Chen, Y., *A simple small molecule as the acceptor for fullerene-free organic solar cells*. Science China Chemistry, 60(3), p.366, (2017).
74. Zhang, H., **Liu, Y.**, Sun, Y., Li, M., Kan, B., Ke, X., Zhang, Q., Wan, X. and Chen, Y., *Developing high-performance small molecule organic solar cells via a large planar structure and an electron-withdrawing central unit*. Chemical Communications, 53(2), p.451, (2017).
75. **Liu, Y.**, Zhang, H., Sun, Y., Wan, X. and Chen, Y., *ADA-type small molecular acceptor with one hexyl-substituted thiophene as π bridge for fullerene-free organic solar cells*. Science China Materials, 60(1), p.49, (2017).

76. Li, M., **Liu, Y. (co-first author)**, Ni, W., Liu, F., Feng, H., Zhang, Y., Liu, T., Zhang, H., Wan, X., Kan, B., Zhang, Q., Russell, T.P., and Chen, Y., *A simple small molecule as an acceptor for fullerene-free organic solar cells with efficiency near 8%*. Journal of Materials Chemistry A, 4(27), p.10409, (2016).
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78. Li, M., Ni, W., Feng, H., Wan, X., **Liu, Y.**, Zuo, Y., Kan, B., Zhang, Q. and Chen, Y., *A low bandgap carbazole based small molecule for organic solar cells*. Organic Electronics, 24, p.89, (2015).

PATENTS AND INVENTION DISCLOSURE

1. Patent: Ievlev, A. V., Ovchinnikova, O. S., Lorenz, M., & Yongtao, LIU. “Time-resolved chemical studies via time-of-flight secondary ion mass spectrometry”, (2022). U.S. Patent No. 11,355,336. Washington, DC: U.S. Patent and Trademark Office.
2. Patent: Ziatdinov, M.Z., Roccapiore, K., Yongtao, LIU., Kelley, K.P., Vasudevan, R.K., Hinkle, J.D., Kalinin, S.V., “Science-driven automated experiments”, (2024). U.S. Patent No. 11,982,684.
3. Invention Disclosure: Kalinin, S.V., Yongtao, LIU, Biswas, A., Duscher, G., Pratiush, U., Roccapiore, K., Ziatdinov, M., Vasudevan, R.K., Valleti, M., Ahmadi, M., “Human-in-the-loop automated experiment”, (2024), Patent ID 81950302
4. Invention Disclosure: “Hypothesis learning in automated experiment: application to combinatorial materials libraries”, Ziatdinov, M., Kalinin, S.V., Yongtao, LIU, (2024), Patent ID 81934321

CONFERENCE PRESENTATIONS

1. (upcoming) **Invited Talk**: Scientific Exploration with Expert Knowledge (SEEK) in Active Learning Powered Autonomous Microscopy; EMA 2025: Basic Science and Electronics Division Meeting, Feb 25-28, 2025, Denver, CO, USA
2. (upcoming) **Invited Talk**: Gated Active Learning for Scientific Exploration in Autonomous Experiments; 2024 APS Mid-Atlantic Section Meeting, Nov 15-17, 2024, Philadelphia, PA, USA
3. **Invited Talk**: *AEcroscopy—Empowering Microscopy Toward Automated and Autonomous Experimentation*; MS&T 2024, Oct 6-9, 2024, Pittsburgh, PA, USA
4. **Invited Talk**: *Navigating the Microscopic World--Autonomous Measurements Powered by Machine Learning*; MLM 2024, Sep 17-19, 2024, Kanazawa, Japan
5. **Invited Seminar Talk**: *The Synergy of AI efficiency and Human Expertise in Autonomous Experimentation*; George and Dot Bishop Advanced Materials Colloquium, Clemson University, Sep 5, 2024
6. Talk: Advancing Microscopy through the Synergy of Human Expertise, LLM efficiency, and API Enabled Automation; 2024 Microscopy and Microanalysis meeting, July 28-Aug 1, 2024, Cleveland, OH, USA.
7. **Invited Talk**: *Navigating the Microscopic World--Autonomous Measurements Powered by Machine Learning*; 78th STLE Annual Meeting; May 19-23, 2024, Minneapolis, MN, USA

8. Talk: *Advancing Microscopy with Machine Learning for Physics Discovery*; EMA 2024 Basic Science and Electronics Division Meeting; Feb 13-16, 2024; Denver, CO, USA
9. Talk: *Harnessing Automation and Machine Learning in Scanning Probe Microscopy to Accelerate Physics Discovery*; 2024 APS March meeting; March 3-8, 2024; Minneapolis, MN, USA
10. Talk: *Automated Microscopy for Physics Discovery*; 2023 MRS Fall Meeting; Nov 26-Dec 1, 2023; Boston, MA, USA
11. Talk: *Automated Microscopy for Physics Discovery: From High Throughput to Hypothesis Learning*; 2023 AVS International Symposium and Exhibition; Nov 5-10, 2023; Portland, OR, USA
12. Talk: *Machine Learning-Driven Autonomous Microscopy for Materials and Physics Discovery*; 2023 Microscopy and Microanalysis, July 23-27, 2023; Minneapolis, MN, USA
13. **Invited Talk:** *Machine Learning Driven Automated Scanning Probe Microscopy for Physics Discovery*; 2023 ACA Annual Meeting, July 7-11, 2023; Baltimore, Maryland, USA
14. Talk: *Study of hybrid perovskite by active learning and ensembled DCNN powered autonomous scanning probe microscopy*; 2023 TechConnect World, June 19-21, 2023; Washington DC, USA.
15. **Invited Talk:** *Machine Learning Driven Automated Scanning Probe Microscopy for Material Discovery: Applications in Ferroelectric and Optoelectronic Materials*; APS March Meeting, March 5-10, 2023; Las Vegas, NV, USA.
16. **Invited Talk:** *Autonomous Scanning Probe Microscopy: From Streaming Image Analysis to Learning Physics*; AVS meeting; November 6-11, 2022; Pittsburgh, PA, USA.
17. **Invited Talk:** *Machine Learning Driven Automated Scanning Probe Microscopy for Materials Discovery*; Seagate AI/ML Distinguished Speaker Series; Oct 7, 2022; Virtual
18. **Invited Talk:** *Machine Learning Driven Automated Microscopy for Materials Discovery*; 2022 SPIE Optics + Photonics; August 21-25, 2022; San Diego, USA.
19. **Invited Talk:** *Machine Learning-Driven Automated SPM: Applications in Ferroelectrics*; 2022 RMS AFM & SPM Meeting; July 4-6, 2022; Hybrid Virtual and In-Person Conference
20. Talk: *Exploring Fundamental Mechanisms of Polarization Switching via Piezoresponse Force Spectroscopy of Composition Spread Libraries*; 2022 ISAF-PFM-ECAPD Joint Conference; June 27-July 1, 2022; Hybrid Virtual and In-Person Conference
21. Talk: *Experimental discovery of structure-property relationships in ferroelectric materials via active learning*; 2022 ISAF-PFM-ECAPD Joint Conference; June 27-July 1, 2022; Hybrid Virtual and In-Person Conference
22. Talk: *Hypothesis-Driven Automated Experiment in Scanning Probe Microscopy: Exploring the Domain Growth Laws in Ferroelectric Materials*; 2022 ISAF-PFM-ECAPD Joint Conference; June 27-July 1, 2022; Hybrid Virtual and In-Person Conference
23. Talk: *Active Learning-Driven Automated Scanning Probe Microscopy Enables Discovery of Structure-Property Relationship*; 2022 APS March Meeting; March 14-18, 2022; Hybrid Virtual and In-Person Conference
24. Poster: *Interface and Bending Effects on Ferroelectricity in Ultrathin CuInP2S6 Probed by Piezoresponse Force Microscopy*; 2022 APS March Meeting; March 14-18, 2022; Hybrid Virtual and In-Person Conference

25. Poster: *Machine Learning-Driven Scanning Probe Microscopy for Ferroelectric Domain Writing*; 2022 APS March Meeting; March 14-18, 2022; Hybrid Virtual and In-Person Conference
26. Talk: *Conductive hotspots in $\text{Hf}_{0.5}\text{Zr}_{0.5}\text{O}_2$: an automated experiment investigation*; 2021 Electronic Materials and Applications; January 19-21, 2021; Virtual Conference
27. **Invited Talk:** *Experimental discovery of structure-property relationships in ferroelectric materials via active learning*; 2022 Electronic Materials and Applications; January 19-21, 2022; Virtual Conference
28. Poster: *Strain in Metal Halide Perovskites: The Critical Role of A-Cation*; 2021 Materials Research Society Fall Meeting; December 6-8, 2021; Hybrid Virtual and In-Person Conference
29. Talk: *Photoinduced iodide repulsion and halides-demixing in layered perovskites*; 2021 Materials Research Society Fall Meeting; December 6-8, 2021; Hybrid Virtual and In-Person Conference
30. Talk: *Decoding the shift-invariant data: applications for band-excitation scanning probe microscopy*; 2021 Materials Research Society Fall Meeting; December 6-8, 2021; Hybrid Virtual and In-Person Conference
31. Talk: *Disentangling ferroelectric wall dynamics and identification of pinning mechanisms via deep learning*; 2021 Materials Research Society Fall Meeting; December 6-8, 2021; Hybrid Virtual and In-Person Conference
32. Talk: *Conductive hotspots in $\text{Hf}_{0.5}\text{Zr}_{0.5}\text{O}_2$: an auto experiment investigation*; 2021 Materials Research Society Fall Meeting; December 6-8, 2021; Hybrid Virtual and In-Person Conference
33. Talk: *Automated Scanning Probe Microscopy Based on Deep Kernel Learning*; 2021 Materials Research Society Fall Meeting; December 6-8, 2021; Hybrid Virtual and In-Person Conference
34. Talk: *Experimental discovery of structure-property relationships in ferroelectric materials via active learning*; 2021 Workshop on Computational and Autonomous Workflows; July 20-21, 2021; Virtual Conference
35. Poster: *Disentangling ferroelectric wall dynamics and identification of pinning mechanisms via deep learning*; 2021 Joint Nanoscience and Neutron Scattering User Meeting; August 2-20, 2021; Virtual Conference.
36. Poster: *Conductive hotspots in $\text{Hf}_{0.5}\text{Zr}_{0.5}\text{O}_2$: an automated experiment investigation*; 2021 Joint Nanoscience and Neutron Scattering User Meeting; August 2-20, 2021; Virtual Conference.
37. **Invited Talk:** *Investigating ferroic behavior of metal halide perovskites*; 2021 Joint ISAF-ISIF-PFM Virtual Conference; May 16-21, 2021; Virtual Conference.
38. Talk: *Subgrain structure and ionic segregation in metal halide semiconductors*; Materials Research Society Spring Meeting; April 17-23, 2021; Virtual Meeting
39. Talk: *Understanding the Chemico-Physical Interactions in Metal Halide Perovskites by Multimodal Imaging Techniques*; Materials Research Society Spring/Fall Meeting; November 27-December 4, 2020; Virtual Conference.

40. Talk: *Operando Imaging of Ion Migration in Metal Halide Perovskite*; Microscopy and Microanalysis 2020 Meeting; August 4-7, 2020; Virtual Conference.
41. Talk: *Hysteretic ion Migration in Methylammonium Lead Iodide*; Materials Research Society Fall Meeting; December 1-6, 2019; Boston, MA, USA.
42. Talk: *Unveiling photoinduced ion dynamics in hybrid organic inorganic perovskites using time-resolved time-of-flight secondary ion mass spectrometry*; Materials Research Society Fall Meeting; December 1-6, 2019; Boston, MA, USA.
43. Talk: *Chemical Dynamics in Hybrid Organic-Inorganic Perovskites*; Materials Research Society Fall Meeting; December 1-6, 2019; Boston, MA, USA. (MRS Graduate Student Silver Award)
44. Talk: *Ferroic-Ionic Interaction in Hybrid Organic-Inorganic Perovskites*; American Vacuum Society 66th International Symposium& Exhibition; October 20-25, 2019; Columbus, OH, USA. (AVS Graduate Research Award)
45. Talk: *Chemical Nature of Ferroelastic Twin Domains in $\text{CH}_3\text{NH}_3\text{PbI}_3$* ; American Vacuum Society 66th International Symposium& Exhibition; October 20-25, 2019; Columbus, OH, USA. (AVS NSTD Division Award Finalist Talk)
46. Talk: *Ferroic-Ionic Interaction in Hybrid Organic-Inorganic Perovskites*; American Vacuum Society 66th International Symposium& Exhibition; October 20-25, 2019; Columbus, OH, USA.
47. Poster: *Ferroic-Ionic Interaction in Hybrid Organic-Inorganic Perovskites*; American Vacuum Society 66th International Symposium& Exhibition; October 20-25, 2019; Columbus, OH, USA.
48. Poster: *Ferroic-Ionic Interaction in Hybrid Organic-Inorganic Perovskites*; Center for Nanophase Materials Sciences User Meeting; August 12-14, 2019; Oak Ridge, TN, USA. (Best Student Poster Award, rank 1st)
49. Talk: *Multi-Modal Imaging of Local Chemistry and Ferroic Properties of Hybrid Organic-Inorganic Perovskites*; Microscopy and Microanalysis 2019 Meeting; August 4-9, 2019; Portland, OR, USA
50. Talk: *Chemical Phenomena in Ferroelastic $\text{CH}_3\text{NH}_3\text{PbI}_3$ Perovskite*; Materials Research Society Fall Meeting; November 25-30, 2018; Boston, MA, USA. (MRS Graduate Student Silver Award)
51. Poster: *Temperature-dependent chemical-structural correlation in MAPbI_3 Perovskite*; Materials Research Society Fall Meeting; November 25-30, 2018; Boston, MA, USA
52. Talk: *Ionic and Electronic Properties of Twin Domain in MAPbI_3* ; Materials Research Society Fall Meeting; November 25-30, 2018; Boston, MA, USA
53. Poster: *Chemical Nature of Ferroelastic Twin Domains in $\text{CH}_3\text{NH}_3\text{PbI}_3$ Perovskite*; Materials Research Society Fall Meeting; November 25-30, 2018; Boston, MA, USA
54. Talk: *Deciphering Chemical Nature of Ferroelastic Twin Domain in MAPbI_3 perovskite by Helium Ion Microscopy Secondary Ion Mass Spectrometry*; American Vacuum Society 65th International Symposium& Exhibition; October 21-26, 2018; Long Beach, CA, USA
55. Poster: *Ionic Activity of Twin Domain in MAPbI_3* ; Center for Nanophase Materials Sciences User Meeting; August 13-15, 2018; Oak Ridge, TN, USA. (Best Student Poster Award)
56. Poster: *Chemical Nature of Ferroelastic Twin Domains in $\text{CH}_3\text{NH}_3\text{PbI}_3$ Perovskite*; Center for Nanophase Materials Sciences User Meeting; August 13-15, 2018; Oak Ridge, TN, USA

57. Poster: *Exploring Ferroelectricity of Hybrid Organic-Inorganic Perovskites*; Materials Research Society Fall Meeting; November 26-December 1, 2017; Boston, MA, USA
58. Poster: *Exploring Ferroelectric/Ferromagnetic Interaction Created by Nickel and Hybrid Organic-Inorganic Perovskites*; Center for Nanophase Materials Sciences User Meeting; July 31-August 3, 2017; Oak Ridge, TN, USA