

Yongtao LIU

Center for Nanophase Materials Science
Oak Ridge National Laboratory, Oak Ridge, TN, USA
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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—2014.06

- BS, College of Chemistry

WORK AND RESEARCH HISTORY

R&D Associate Staff 2023.04—present

- Data NanoAnalytics Group, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee, United States
- Developing automated and autonomous scanning probe microscopy harnessing the power of machine learning for physics and materials discovery.

Postdoctoral Research Associate 2021.04—2023.04

- 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 2016.08—2020.12

- 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.

Graduate Research Assistant 2013.06—2016.06

- Institute of Polymer Chemistry, Nankai University, Tianjin, United States
- Designing and synthesizing organic small molecules for efficient photovoltaics

HONORS AND AWARDS

- **AVS NSTD Early Career Competition Finalist**, American Vacuum Society, 2023
- **R&D 100 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

PROFESSIONAL SERVICE

Society Committee Member

- 2023-2025: Executive Committee Member of American Vacuum Society Nanoscale Science and Technology Division

Conference Symposium and Workshop Organizer

- 2024 MRS Fall Meeting: *Symposium MT02-Machine Learning in Action—Automated and Autonomous Experiments*; Dec 1- 6, 2024; Boston, MA
- 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

Society Membership

- 2023 – present: Member of *American Crystallographic Association (ACA)*
- 2021 – present: Member of *American Ceramic Society (ACerS)*
- 2021 – present: Member of *American Physical Society (APS)*
- 2018 – present: Member of *Materials Research Society (MRS)*
- 2019 – present: Member of *American Vacuum Society (AVS)*
- 2019 – present: Member of *Microanalysis Society (MAS)*

Editorial Service

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

Review Service

- Reviewer for *Advanced Materials*; *Advanced Functional Materials*; *Small*; *Advanced Optical Materials*; *Applied Physics Letters*; *ChemPhysChem*; *Solar Energy*; *Nanoscale*; *Nanotechnology*; *Communication Materials*; *Journal of Materials Science: Materials in*

PUBLICATIONS

- **Google Scholar:** <https://scholar.google.com/citations?user=V9FMPgQAAAAJ&hl=en>
- 1. 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).
- 2. **Liu, Y.***, Roccapiore, K., Checa, M., Valletti, S. M., Yang, J. C., Jesse, S., & Vasudevan, R. K.*. AEcroscPy: A software-hardware framework empowering microscopy toward automated and autonomous experimentation. *arXiv preprint arXiv:2312.10281* (2023).
- 3. 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).
- 4. **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).
- 5. **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).
- 6. 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).
- 7. 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. *arXiv preprint arXiv:2310.06583*, (2023).
- 8. **Liu, Y.***, Ziatdinov, M., Vasudevan, R., and Kalinin, S.V.*. "Explainability and human intervention in autonomous scanning probe microscopy." *Patterns* (2023).
- 9. 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).
- 10. 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. *arXiv preprint arXiv:2310.05018*, (2023).
- 11. 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. *arXiv preprint arXiv:2309.05136*, (2023).
- 12. 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).
- 13. 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).

14. 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).
15. 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).
16. Biswas, A., **Liu, Y.**, Creange, N., Liu, Y. C., Jesse, S., Yang, J. C., Kalinin, S.V., Ziatdinov, M.A., Vasudevan, R. K., “A dynamic Bayesian optimized active recommender system for curiosity-driven Human-in-the-loop automated experiments”. arXiv preprint arXiv:2304.02484, (2023).
17. 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 ferroelectrics. arXiv preprint arXiv:2305.15247, (2023).
18. 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).
19. Mani, V., **Liu, Y.**, and Kalinin, S.V., "Physics and Chemistry from Parsimonious Representations: Image Analysis via Invariant Variational Autoencoders." arXiv preprint arXiv:2303.18236 (2023).
20. Kalinin, S.V., Ziatdinov, M., Ahmadi, M., Ghosh, A., Roccapiore, K., **Liu, Y.**, and Vasudevan, R.K., "Designing Workflows for Materials Characterization." arXiv preprint arXiv:2302.04397 (2023).
21. **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.
22. 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).
23. **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).
24. **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).
25. **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).
26. **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).
27. **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)

28. 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).
29. 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).
30. 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).
31. 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.
32. **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).
33. 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.
34. 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.
35. **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.
36. **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
37. **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*, 2022, DOI:10.1038/s42256-022-00460-0.
38. **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.
39. 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, *arXiv preprint arXiv:2105.11475* (2021).
40. **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).
41. **Liu, Y.**, Kim, D., Ievlev, A. V., Kalinin, S. V., Ahmadi, M., Ovchinnikova, O. S., Ferroic halide perovskite optoelectronics, *Advanced Functional Materials*, 202102793 (2021).
42. 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.
43. **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.
 44. **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).
 45. **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).
 46. **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).
 47. **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).
 48. **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).
 49. 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).
 50. **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).
 51. **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).
 52. 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).
 53. **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).
 54. **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).
 55. **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 CH₃NH₃PbI₃ perovskites. *Nature materials*, 18(10), p.1051, (2019).
56. Collins, L., **Liu, Y.**, Ovchinnikova, O.S., & Proksch, R., Quantitative Electromechanical Atomic Force Microscopy. *ACS Nano*, 13(7), p.8055, (2019).
57. **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 CH₃NH₃PbI₃ perovskite. *Nature materials*, 17(11), p.1013, (2018).
58. **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 CH₃NH₃PbI₃ perovskite twin domains. *Applied Physics Letters*, 113(7), p.072102, (2018).
59. 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).
60. **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).
61. 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).
62. 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).
63. **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).
64. 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).
65. Xu, W., **Liu, Y.**, Huang, X., Jiang, L., Li, Q., Hu, X., Huang, F., Gong, X., and Cao, Y., Solution-processed VOx prepared using a novel synthetic method as the hole extraction layer for polymer solar cells. *Journal of Materials Chemistry C*, 4(10), p.1953, (2016).
66. 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).

CONFERENCE PRESENTATIONS

1. “Automated Microscopy for Physics Discovery”, Talk, 2023 MRS Fall Meeting, Nov 26-Dec 1, 2023, Boston, MA, USA
2. “Automated Microscopy for Physics Discovery: From High Throughput to Hypothesis Learning”, Talk, 2023 AVS International Symposium and Exhibition, Nov 5-10, 2023, Portland, OR, USA

3. “Machine Learning-Driven Autonomous Microscopy for Materials and Physics Discovery”, Talk, 2023 Microscopy and Microanalysis, July 23-27, 2023, Minneapolis, MN, USA
4. “Machine Learning Driven Automated Scanning Probe Microscopy for Physics Discovery”, **Invited Talk**, 2023 ACA Annual Meeting, July 7-11, 2023, Baltimore, Maryland, USA
5. “Study of hybrid perovskite by active learning and ensembled DCNN powered autonomous scanning probe microscopy”, Talk, 2023 TechConnect World, June 19-21, 2023, Washington DC, USA.
6. “Machine Learning Driven Automated Scanning Probe Microscopy for Material Discovery: Applications in Ferroelectric and Optoelectronic Materials”, **Invited Talk**, APS March Meeting, March 5-10, 2023, Las Vegas, NV, USA.
7. “Autonomous Scanning Probe Microscopy: From Streaming Image Analysis to Learning Physics”, **Invited Talk**, AVS meeting, November 6-11, 2022, Pittsburgh, PA, USA.
8. “Machine Learning Driven Automated Scanning Probe Microscopy for Materials Discovery”, **Invited Talk**, Seagate AI/ML Distinguished Speaker Series, Oct 7, 2022, Virtual
9. “Machine Learning Driven Automated Microscopy for Materials Discovery”, **Invited Talk**, 2022 SPIE Optics + Photonics, August 21-25, 2022 San Diego, USA.
10. “Machine Learning-Driven Automated SPM: Applications in Ferroelectrics”, **Invited Talk**, 2022 RMS AFM &SPM Meeting, July 4-6, 2022, Hybrid Virtual and In-Person Conference
11. “Exploring Fundamental Mechanisms of Polarization Switching via Piezoresponse Force Spectroscopy of Composition Spread Libraries”, Talk, 2022 ISAF-PFM-ECAPD Joint Conference, June 27-July 1, 2022, Hybrid Virtual and In-Person Conference
12. “Experimental discovery of structure-property relationships in ferroelectric materials via active learning”, Talk, 2022 ISAF-PFM-ECAPD Joint Conference, June 27-July 1, 2022, Hybrid Virtual and In-Person Conference
13. “Hypothesis-Driven Automated Experiment in Scanning Probe Microscopy: Exploring the Domain Growth Laws in Ferroelectric Materials”, Talk, 2022 ISAF-PFM-ECAPD Joint Conference, June 27-July 1, 2022, Hybrid Virtual and In-Person Conference
14. “Active Learning-Driven Automated Scanning Probe Microscopy Enables Discovery of Structure-Property Relationship”, Talk, 2022 APS March Meeting, March 14-18, 2022, Hybrid Virtual and In-Person Conference
15. “Interface and Bending Effects on Ferroelectricity in Ultrathin CuInP_2S_6 Probed by Piezoresponse Force Microscopy”, Poster, 2022 APS March Meeting, March 14-18, 2022, Hybrid Virtual and In-Person Conference
16. “Machine Learning-Driven Scanning Probe Microscopy for Ferroelectric Domain Writing”, Poster, 2022 APS March Meeting, March 14-18, 2022, Hybrid Virtual and In-Person Conference
17. “Conductive hotspots in $\text{Hf}_0.5\text{Zr}_0.5\text{O}_2$: an automated experiment investigation”, Talk, 2021 Electronic Materials and Applications, January 19-21, 2021, Virtual Conference
18. “Experimental discovery of structure-property relationships in ferroelectric materials via active learning”, **Invited talk**, 2022 Electronic Materials and Applications, January 19-21, 2022, Virtual Conference

19. "Strain in Metal Halide Perovskites: The Critical Role of A-Cation", Poster, 2021 Materials Research Society Fall Meeting, December 6-8, 2021, Hybrid Virtual and In-Person Conference
20. "Photoinduced iodide repulsion and halides-demixing in layered perovskites", Talk, 2021 Materials Research Society Fall Meeting, December 6-8, 2021, Hybrid Virtual and In-Person Conference
21. "Decoding the shift-invariant data: applications for band-excitation scanning probe microscopy", Talk, 2021 Materials Research Society Fall Meeting, December 6-8, 2021, Hybrid Virtual and In-Person Conference
22. "Disentangling ferroelectric wall dynamics and identification of pinning mechanisms via deep learning", Talk, 2021 Materials Research Society Fall Meeting, December 6-8, 2021, Hybrid Virtual and In-Person Conference
23. "Conductive hotspots in $\text{Hf}_{0.5}\text{Zr}_{0.5}\text{O}_2$: an auto experiment investigation", Talk, 2021 Materials Research Society Fall Meeting, December 6-8, 2021, Hybrid Virtual and In-Person Conference
24. "Automated Scanning Probe Microscopy Based on Deep Kernel Learning", Talk, 2021 Materials Research Society Fall Meeting, December 6-8, 2021, Hybrid Virtual and In-Person Conference
25. "Experimental discovery of structure-property relationships in ferroelectric materials via active learning", Talk, 2021 Workshop on Computational and Autonomous Workflows, July 20-21, 2021, Virtual Conference
26. "Disentangling ferroelectric wall dynamics and identification of pinning mechanisms via deep learning", Poster, 2021 Joint Nanoscience and Neutron Scattering User Meeting, August 2-20, 2021, Virtual Conference.
27. "Conductive hotspots in $\text{Hf}_{0.5}\text{Zr}_{0.5}\text{O}_2$: an automated experiment investigation", Poster, 2021 Joint Nanoscience and Neutron Scattering User Meeting, August 2-20, 2021, Virtual Conference.
28. "Investigating ferroic behavior of metal halide perovskites", **Invited talk**, 2021 Joint ISAF-ISIF-PFM Virtual Conference, May 16-21, 2021, Virtual Conference.
29. "Subgrain structure and ionic segregation in metal halide semiconductors", Talk, Materials Research Society Spring Meeting, April 17-23, 2021, Virtual Meeting
30. "Understanding the Chemico-Physical Interactions in Metal Halide Perovskites by Multimodal Imaging Techniques", Talk, Materials Research Society Spring/Fall Meeting, November 27-December 4, 2020, Virtual Conference.
31. "Operando Imaging of Ion Migration in Metal Halide Perovskite", Talk, Microscopy and Microanalysis 2020 Meeting, August 4-7, 2020, Virtual Conference.
32. "Hysteretic ion Migration in Methylammonium Lead Iodide", Talk, Materials Research Society Fall Meeting, December 1-6, 2019, Boston, MA, USA.
33. "Unveiling photoinduced ion dynamics in hybrid organic inorganic perovskites using time-resolved time-of-flight secondary ion mass spectrometry", Talk, Materials Research Society Fall Meeting, December 1-6, Boston, MA, USA.
34. "Chemical Dynamics in Hybrid Organic-Inorganic Perovskites", Talk, Materials Research Society Fall Meeting, December 1-6, Boston, MA, USA. (MRS Graduate Student Silver Award)

35. "Ferroic-Ionic Interaction in Hybrid Organic-Inorganic Perovskites", Talk, American Vacuum Society 66th International Symposium& Exhibition, October 20-25, 2019, Columbus, OH, USA. (AVS Graduate Research Award)
36. "Chemical Nature of Ferroelastic Twin Domains in $\text{CH}_3\text{NH}_3\text{PbI}_3$ ", Talk, American Vacuum Society 66th International Symposium& Exhibition, October 20-25, 2019, Columbus, OH, USA. (AVS NSTD Division Award Finalist Talk)
37. "Ferroic-Ionic Interaction in Hybrid Organic-Inorganic Perovskites", Talk, American Vacuum Society 66th International Symposium& Exhibition, October 20-25, 2019, Columbus, OH, USA. (Poster Flash Talk)
38. "Ferroic-Ionic Interaction in Hybrid Organic-Inorganic Perovskites", Poster, American Vacuum Society 66th International Symposium& Exhibition, October 20-25, 2019, Columbus, OH, USA.
39. "Ferroic-Ionic Interaction in Hybrid Organic-Inorganic Perovskites", Poster, Center for Nanophase Materials Sciences User Meeting, August 12-14, 2019, Oak Ridge, TN, USA. (Best Student Poster Award, rank 1st)
40. "Multi-Modal Imaging of Local Chemistry and Ferroic Properties of Hybrid Organic-Inorganic Perovskites", Talk, Microscopy and Microanalysis 2019 Meeting, August 4-9, 2019, Portland, OR, USA
41. "Chemical Phenomena in Ferroelastic $\text{CH}_3\text{NH}_3\text{PbI}_3$ Perovskite", Talk, Materials Research Society Fall Meeting, November 25-30, 2018, Boston, MA, USA. (MRS Graduate Student Silver Award)
42. "Temperature-dependent chemical-structural correlation in MAPbI_3 Perovskite", Poster, Materials Research Society Fall Meeting, November 25-30, 2018, Boston, MA, USA
43. "Ionic and Electronic Properties of Twin Domain in MAPbI_3 ", Talk, Materials Research Society Fall Meeting, November 25-30, 2018, Boston, MA, USA
44. "Chemical Nature of Ferroelastic Twin Domains in $\text{CH}_3\text{NH}_3\text{PbI}_3$ Perovskite", Poster, Materials Research Society Fall Meeting, November 25-30, 2018, Boston, MA, USA
45. "Deciphering Chemical Nature of Ferroelastic Twin Domain in MAPbI_3 perovskite by Helium Ion Microscopy Secondary Ion Mass Spectrometry", Talk, American Vacuum Society 65th International Symposium& Exhibition, October 21-26, 2018, Long Beach, CA, USA
46. "Ionic Activity of Twin Domain in MAPbI_3 ", Poster, Center for Nanophase Materials Sciences User Meeting, August 13-15, 2018, Oak Ridge, TN, USA. (Best Student Poster Award)
47. "Chemical Nature of Ferroelastic Twin Domains in $\text{CH}_3\text{NH}_3\text{PbI}_3$ Perovskite", Poster, Center for Nanophase Materials Sciences User Meeting, August 13-15, 2018, Oak Ridge, TN, USA
48. "Exploring Ferroelectricity of Hybrid Organic-Inorganic Perovskites", Poster, Materials Research Society Fall Meeting, November 26-December 1, 2017, Boston, MA, USA
49. "Exploring Ferroelectric/Ferromagnetic Interaction Created by Nickel and Hybrid Organic-Inorganic Perovskites", Poster, Center for Nanophase Materials Sciences User Meeting, July 31-August 3, 2017, Oak Ridge, TN, USA