Curriculum Vitae

Maxim Ziatdinov, Ph.D.

R&D Staff Scientist
Computational Sciences and Engineering Division
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My research is directed primarily toward the synergy of experiment, theory, and machine learning for accelerated scientific discovery. I am particularly interested in developing physics-based machine learning approaches to enable 'smart labs' of the future. I have pioneered the development of AI-guided autonomous experimentation in microscopy ('self-driving microscopes') and developed the hypothesis learning framework for co-navigation of the hypothesis and experimental spaces in automated experiments.

Professional Experience:

2022-present	Team Lead, Autonomous Scanning Transmission Electron Microscopy project, INTERSECT initiative at Oak Ridge National Laboratory
2021-present	R&D Staff, Computational Sciences and Engineering Division, Oak Ridge National Laboratory
2018-2021	R&D Associate, Computational Sciences and Engineering Division, Oak Ridge National Laboratory
2015-2018	Postdoctoral Research Associate, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory

Education:

Tokyo Institute of Technology	Materials Science and Engineering	Ph.D. 2014
Tokyo Institute of Technology	Materials Science and Engineering	M.S. 2011
Far Eastern National University	Physics and Microelectronics	B.A. 2009

Book chapters:

1. S. V. Kalinin, E. Strelcov, R. K. Vasudevan, M. Ziatdinov, "Big and Deep Data Methods in Scanning Probe Microscopy and Spectroscopy", in *Handbook on Big Data and Machine Learning in the Physical Sciences*, World Scientific, 2020, pp. 301–362.
2. A. Maksov, S. V. Kalinin, R. K. Vasudevan, M. Ziatdinov, "Deep Machine Learning in Electron and Scanning Probe Microscopy", in *Handbook on Big Data and Machine Learning in the Physical Sciences*, World Scientific, 2020, pp. 363–395.
3. M. Ziatdinov, A. Maksov, S. V. Kalinin, "Deep Data Analytics in Structural and Functional Imaging of Nanoscale Material", in *Materials Discovery and Design: By Means of Data Science and Optimal Learning*, Springer International Publishing, Cham, 2018, pp. 103–128.

Selected peer-reviewed publications:
(full list available via Google Scholar)

1. M. Ziatdinov, Y. Liu, A. N. Morozovska, E. A. Eliseev, X. Zhang, I. Takeuchi, S. V. Kalinin. Hypothesis Learning in Automated Experiment: Application to Combinatorial Materials Libraries. *Advanced Materials* 2201345 (2022).
2. Y. Liu, K. P. Kelley, R. K. Vasudevan, H. Funakubo, M. Ziatdinov, S. V. Kalinin. Experimental discovery of structure–property relationships in ferroelectric materials via active learning. *Nature Machine Intelligence* **4,** 341–350 (2022).

3. R. K. Vasudevan, K. P. Kelley, J. Hinkle, H. Funakubo, S. Jesse, S. V. Kalinin, M. Ziatdinov. Autonomous Experiments in Scanning Probe Microscopy and Spectroscopy: Choosing Where to Explore Polarization Dynamics in Ferroelectrics. *ACS Nano 15*, 11253-11262 (2021).
4. A. Ghosh, B. G. Sumpter, O. Dyck, S. V. Kalinin, M. Ziatdinov. Ensemble learning-iterative training machine learning for uncertainty quantification and automated experiment in atom-resolved microscopy. *npj Comput Mater* **7**, 100 (2021).
5. S. V. Kalinin, O. Dyck, S. Jesse, M. Ziatdinov. Exploring order parameters and dynamic processes in disordered systems via variational autoencoders. *Science Advances* **7**, eabd5084 (2021).
6. S. V. Kalinin, S. Zhang, M. Valleti, H. Pyles, D. Baker, J. J. De Yoreo, M. Ziatdinov. Disentangling Rotational Dynamics and Ordering Transitions in a System of Self-Organizing Protein Nanorods via Rotationally Invariant Latent Representations. *ACS Nano* **15**, 6471-6480 (2021).
7. S. V. Kalinin, K. Kelley, R. K. Vasudevan, M. Ziatdinov. Toward Decoding the Relationship between Domain Structure and Functionality in Ferroelectrics via Hidden Latent Variables. *ACS Appl. Mater. Interfaces*. **13**, 1693–1703 (2021).
8. M. Ziatdinov, N. Creange, X. Zhang, A. Morozovska, E. Eliseev, R. K. Vasudevan, I. Takeuchi, C. Nelson, S. V. Kalinin. Predictability as a probe of manifest and latent physics: The case of atomic scale structural, chemical, and polarization behaviors in multiferroic Sm-doped $BiFeO_3$. *Applied Physics Reviews*. **8**, 011403 (2021).
9. M. Ziatdinov, S. Jesse, B. G. Sumpter, S. V. Kalinin, O. Dyck, Tracking atomic structure evolution during directed electron beam induced Si-atom motion in graphene via deep machine learning. *Nanotechnology* **32**, 035703 (2020).
10. S. V. Kalinin, M. Valleti, R. K. Vasudevan, M. Ziatdinov. Exploration of lattice Hamiltonians for functional and structural discovery via Gaussian process-based exploration–exploitation. *Journal of Applied Physics* **128**, 164304 (2020).
11. M. Ziatdinov, C. T. Nelson, X. Zhang, R. K. Vasudevan, E. Eliseev, A. N. Morozovska, I. Takeuchi and S. V. Kalinin. Causal analysis of competing atomistic mechanisms in ferroelectric materials from high-resolution scanning transmission electron microscopy data. *npj Computational Materials* **6** (1), 127 (2020).
12. M. Ziatdinov, D. Kim, S. Neumayer, R. K. Vasudevan, L. Collins, S. Jesse, M. Ahmadi, S. V. Kalinin, Imaging mechanism for hyperspectral scanning probe microscopy via Gaussian process modelling. *npj Computational Materials*. **6**, 21 (2020).
13. M. Ziatdinov, O. Dyck, X. Li, B. G. Sumpter, S. Jesse, R. K. Vasudevan, S. V. Kalinin, Building and exploring libraries of atomic defects in graphene: Scanning transmission electron and scanning tunneling microscopy study. *Science Advances* **5**, eaaw8989 (2019).

Open-Source Software Development:

- Creator and lead developer of AtomAI software library for deep/machine learning analysis of microscopy data (https://github.com/pycroscopy/atomai).
- Creator and lead developer of GPax software package for physics-based Gaussian processes and Bayesian optimization (https://github.com/ziatdinovmax/gpax).
- Creator and lead developer of pyroVED software package for applications of variational autoencoders in image and spectral analyses (https://github.com/ziatdinovmax/pyroved).

Honors & Awards:

Foresight Institute Fellowship 2021
Microscopy Today Innovation Award 2019
Oak Ridge National Laboratory Significant Event Award 2018
Japanese Government (MEXT) Scholarship 2009-2014
Murata Science Foundation Travel Fellowship 2013
Student Award at International Conference “Carbon 2008” (Nagano, Japan)