*Curriculum Vitae*

# Maxim Ziatdinov, Ph.D.

R&D Staff Scientist
Computational Sciences and Engineering Division
& Center for Nanophase Materials Sciences
Oak Ridge National Laboratory
E-mail: ziatdinovma@ornl.gov

My research is directed primarily toward the synergy of experiment, theory, and machine learning for accelerated discoveries in the fields of materials science and nanoscience. I am particularly interested in the development of physics-based machine learning approaches for analyzing complex molecular, atomic, and electronic patterns from scanning probe and electron microscopy experiments on classical and quantum materials. In addition, I am working on the machine learning-enabled "smart" automation of imaging and spectroscopic instrumentation.

**Education:**

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|---|---|---|
| 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 |

**Research and Professional Experience:**

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, Scanning Probe Microscopy Group, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory

**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. 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* (2021), in print. DOI: 10.1021/acsnano.0c10239.

2. 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).

3.  S. V. Kalinin, O. Dyck, S. Jesse, <u>M. Ziatdinov</u>. Exploring order parameters and dynamic processes in disordered systems via variational autoencoders. *Science Advances* **7**, eabd5084 (2021).
4.  S. V. Kalinin, S. Zhang, M. Valleti, H. Pyles, D. Baker, J. J. De Yoreo, <u>M. Ziatdinov</u>. 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).
5.  S. V. Kalinin, K. Kelley, R. K. Vasudevan, <u>M. Ziatdinov</u>. Toward Decoding the Relationship between Domain Structure and Functionality in Ferroelectrics via Hidden Latent Variables. *ACS Appl. Mater. Interfaces*. **13**, 1693–1703 (2021).
6.  <u>M. Ziatdinov</u>, 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).
7.  <u>M. Ziatdinov</u>, 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).
8.  S. V. Kalinin, M. Valleti, R. K. Vasudevan, <u>M. Ziatdinov</u>. Exploration of lattice Hamiltonians for functional and structural discovery via Gaussian process-based exploration–exploitation. *Journal of Applied Physics* **128**, 164304 (2020).
9.  <u>M. Ziatdinov</u>, 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).
10. K. Kelley, <u>M. Ziatdinov</u>, L. Collins, M. A. Susner, R. K. Vasudevan, N. Balke, S. V. Kalinin, S. Jesse. Fast Scanning Probe Microscopy via Machine learning: Non-Rectangular Scans with Compressed Sensing and Gaussian Process Optimization. *Small* **16**, 2002878 (2020).
11. <u>M. Ziatdinov</u>, 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).
12. <u>M. Ziatdinov</u>, 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 GPim software package for application of Gaussian processes and Bayesian optimization to imaging and spectroscopic datasets (https://github.com/ziatdinovmax/GPim).
- Creator and lead developer of pyroVED software package for applications of variational autoencoders in image and spectral analyses (https://github.com/ziatdinovmax/pyroved).
- Active contributor to various packages in the Pycroscopy ecosystem (https://github.com/pycroscopy), including packages for storing and visualization of high-dimensional imaging and spectroscopic data.


**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
Russian Foundation for Basic Research Young Scientist Travel Grant 2009
Student Award at International Conference "Carbon 2008" (Nagano, Japan)