Curriculum Vitae

Maxim Ziatdinov, Ph.D.

R&D Scientist
Computational Sciences and Engineering Division
& Center for Nanophase Materials Sciences
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My expertise lies in designing and implementing custom machine learning solutions that drive research and development. With a proven track record of collaborating closely with academic and industry partners, I excel at translating complex domain-specific challenges into efficient machine learning codes and workflows. My achievements include leading the development of AI-driven autonomous experimentation in scanning probe and electron microscopy ("self-driving microscopes") and creating a hypothesis learning framework that enables science-informed automated experimentation. To support my peers, I have authored multiple widely used open-source software packages, such as AtomAI, which streamlines machine learning integration into experimental research. I also introduced the Jupyter paper concept to enhance transparency and reproducibility in research. My vision for the future of R&D is one where smart labs powered by machine learning are the norm, and where human intelligence is augmented by data-driven insights.

Skills & Expertise: Deep Learning (PyTorch, TensorFlow, JAX), Probabilistic Programming (Pyro, PyMC), Materials Sciences (quantum, energy, functional), Imaging Experiments (AFM, (S)TEM, STM), Edge Computing (NVIDIA Jetsons)

PROFESSIONAL EXPERIENCE:

Project Lead | Autonomous Electron Microscopy
Oak Ridge National Laboratory | March 2022 – present

- Led a cross-functional team of imaging, simulation, and machine learning researchers to achieve project goals and objectives.
- Spearheaded the development of machine learning workflows for on-the-fly analysis of streaming data for feedback and instrument control.
- Oversaw the establishment of critical links between cutting-edge instrumental platforms and high-performance computing facilities to optimize data processing and analysis.

R&D Scientist
Oak Ridge National Laboratory | May 2018 – present

- Developed hypothesis learning framework that combines structured Gaussian processes with Reinforcement Learning policies to guide experiments (synthesis, microscopy) on understanding cooperative phenomena in functional materials.
- Created machine learning pipelines that leverage convolutional neural networks, mixture modelling, and graph analysis to direct electron beam-induced nanoscale transformations for quantum device fabrication.
- Designed custom variational autoencoders for unsupervised learning of physically-meaningful disentangled representations from imaging and spectroscopic datasets on classical and quantum materials.
- Worked with academia and industry researchers to translate their domain-specific problems into machine learning codes and workflows at the Center for Nanophase Materials Sciences, a scientific user facility of the Department of Energy.

Postdoctoral Research Associate
Oak Ridge National Laboratory | Feb 2015 – May 2018

- Cryogenic ultra-high vacuum scanning tunneling microscopy measurements of quantum materials.
- Pioneered successful application of deep neural networks to imaging data from electron and scanning probe microscopy experiments.

MACHINE LEARNING SOFTWARE DEVELOPMENT:

- Creator of the AtomAI software framework for deep and machine learning analysis of microscopy data (https://github.com/pycroscopy/atomai) *~80k downloads*.
  Featured by C&EN in *Computers Are Learning How to Analyze Chemist's Spectra and Micrographs*
- Creator of the GPax software package for structured Gaussian processes and deep kernel active learning (https://github.com/ziatdinovmax/gpax) *~5k downloads*.
- Creator of the pyroVED software package for applications of invariant variational autoencoders in image and spectral analyses (https://github.com/ziatdinovmax/pyroved) *~16k downloads*.

SELECTED PEER-REVIEWED PUBLICATIONS:
(total publications > 80, citations > 2400, h-index = 26, see full list on Google Scholar)

1. M. Ziatdinov, A. Ghosh, T. Wong, S. V. Kalinin. *AtomAI: A Framework for Deep Learning Analysis of Image and Spectroscopy Data in Electron and Scanning Probe Microscopy*. **Nature Machine Intelligence** 4, 1101-1112 (2022).
This paper introduces our in-house built AtomAI software framework for bridging instrument-specific libraries, deep learning and simulation tools into a single ecosystem and illustrates its applications for various imaging and spectroscopic experiments.
2. S. V. Kalinin, A. Ghosh, R. K. Vasudevan, M. Ziatdinov. *From Atomically Resolved Imaging to Generative and Causal Models*. **Nature Physics** 18, 1152-1160 (2022).
This paper explores the possibility of AI-driven extraction of domain-specific information from microscopy data toward building generative models for a broader parameter space and exploring causal mechanisms underpinning functionalities.
3. M. Ziatdinov, A. Ghosh, S. V. Kalinin. *Physics makes the difference: Bayesian optimization and active learning via augmented Gaussian process*. **Machine Learning: Science and Technology** 3, 015003 (2022).
Here we introduced a methodology for injecting prior knowledge in the form of physical/phenomenological models into the Bayesian optimization framework by augmenting the Gaussian process with a probabilistic model of expected system's behavior.
4. K. Roccapriore, S. V. Kalinin, M. Ziatdinov. *Physics Discovery in Nanoplasmonic Systems via Autonomous Experiments in Scanning Transmission Electron Microscopy*. **Advanced Science** 9, 2203422 (2022).
In this paper, we demonstrated the first realization of "self-driving" electron microscopy where deep kernel (active) learning was used to explore structure-property relationships in materials in an automated fashion.
5. 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, 127 (2020).
This paper demonstrated the first application of causal inference to materials science problem, examining the interplay between physical and chemical effects across the ferroelectric–antiferroelectric phase transitions in real materials.
6. 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).
Here we demonstrated a Gaussian process-based approach for rapid exploration of the phase diagrams based on specific thermodynamic or structural parameters of interest for models ranging from simple lattice to complex quantum Hamiltonians.

EDUCATION:

Sep 2014	PhD, Materials Sciences and Engineering	Tokyo Institute of Technology
Sep 2011	MS, Materials Sciences and Engineering	Tokyo Institute of Technology
June 2009	MS, Physics and Microelectronics	Far Eastern National University

SERVICE TO COMMUNITY:
AI/ML workshop organizer:
- "*AI for Atoms: How to Machine Learn STEM*" (> 250 participants)
- "*Machine Learning and Automated Experiments in Scanning Probe Microscopy*" (>100 participants)

Editorial Board Member: *npj Computational Materials (Nature Partner Journal)*, *Journal of Materials Informatics*.
Reviewer: *Journal of Open-Source Software, Nature Materials, Science Advances, Journal of American Chemical Society*, *ACS Nano, Nano Letters*, *Digital Discovery*, *and others*.

INVITED TALKS:
American Physical Society (2019, 2023), Microscopy & Microanalysis (2023), Monterey Data Conference (2019), UC Berkeley/LBNL (2018, 2019, 2023), Institute for Pure and Applied Mathematics (2023x2), MIT (2022)

AWARDS:
Oak Ridge National Laboratory Outstanding Scholarly Output 2022
Microscopy Today Innovation Award 2019: *AICrystallographer*

RESEARCH HIGHLIGHTS:
IEEE Spectrum: Self-Driving Microscopes to Navigate the Nanoscale
C&EN: Computers Are Learning How to Analyze Chemist's Spectra and Micrographs
ORNL News: Awards night recipient streamlines materials synthesis with automation, machine learning
ORNL News: Self-driving microscopes discover shortcuts to new materials
ORNL News: Automated chemistry sets new pace for materials discovery