

Maxim A Ziatdinov

List of Publications by Year in descending order

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111
papers

2,329
citations

218592

26
h-index

243529

44
g-index

116
all docs

116
docs citations

116
times ranked

2327
citing authors

#	ARTICLE	IF	CITATIONS
1	Deep Learning of Atomically Resolved Scanning Transmission Electron Microscopy Images: Chemical Identification and Tracking Local Transformations. ACS Nano, 2017, 11, 12742-12752.	7.3	282
2	Deep learning analysis of defect and phase evolution during electron beam-induced transformations in WS ₂ . Npj Computational Materials, 2019, 5, .	3.5	113
3	Materials science in the artificial intelligence age: high-throughput library generation, machine learning, and a pathway from correlations to the underpinning physics. MRS Communications, 2019, 9, 821-838.	0.8	109
4	Learning surface molecular structures via machine vision. Npj Computational Materials, 2017, 3, .	3.5	79
5	Atom-by-atom fabrication with electron beams. Nature Reviews Materials, 2019, 4, 497-507.	23.3	73
6	Building and exploring libraries of atomic defects in graphene: Scanning transmission electron and scanning tunneling microscopy study. Science Advances, 2019, 5, eaaw8989.	4.7	70
7	Atomic-scale observation of structural and electronic orders in the layered compound $\hat{1}\pm$ -RuCl ₃ . Nature Communications, 2016, 7, 13774.	5.8	66
8	Chemical Robotics Enabled Exploration of Stability in Multicomponent Lead Halide Perovskites via Machine Learning. ACS Energy Letters, 2020, 5, 3426-3436.	8.8	66
9	Machine learning in scanning transmission electron microscopy. Nature Reviews Methods Primers, 2022, 2, .	11.8	59
10	Role of edge geometry and chemistry in the electronic properties of graphene nanostructures. Faraday Discussions, 2014, 173, 173-199.	1.6	58
11	Automated and Autonomous Experiments in Electron and Scanning Probe Microscopy. ACS Nano, 2021, 15, 12604-12627.	7.3	49
12	Deep data analysis via physically constrained linear unmixing: universal framework, domain examples, and a community-wide platform. Advanced Structural and Chemical Imaging, 2018, 4, 6.	4.0	45
13	Direct imaging of monovacancy-hydrogen complexes in a single graphitic layer. Physical Review B, 2014, 89, .	1.1	44
14	Bowl Inversion and Electronic Switching of Buckybowls on Gold. Journal of the American Chemical Society, 2016, 138, 12142-12149.	6.6	44
15	Machine learning for high-throughput experimental exploration of metal halide perovskites. Joule, 2021, 5, 2797-2822.	11.7	44
16	Visualization of electronic states on atomically smooth graphitic edges with different types of hydrogen termination. Physical Review B, 2013, 87, .	1.1	41
17	Phases and Interfaces from Real Space Atomically Resolved Data: Physics-Based Deep Data Image Analysis. Nano Letters, 2016, 16, 5574-5581.	4.5	40
18	Exploring order parameters and dynamic processes in disordered systems via variational autoencoders. Science Advances, 2021, 7, .	4.7	38

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19	Fast Scanning Probe Microscopy via Machine Learning: Non-Rectangular Scans with Compressed Sensing and Gaussian Process Optimization. <i>Small</i> , 2020, 16, e2002878.	5.2	37
20	Experimental discovery of structure-property relationships in ferroelectric materials via active learning. <i>Nature Machine Intelligence</i> , 2022, 4, 341-350.	8.3	37
21	High-Throughput Study of Antisolvents on the Stability of Multicomponent Metal Halide Perovskites through Robotics-Based Synthesis and Machine Learning Approaches. <i>Journal of the American Chemical Society</i> , 2021, 143, 19945-19955.	6.6	35
22	Toward Electrochemical Studies on the Nanometer and Atomic Scales: Progress, Challenges, and Opportunities. <i>ACS Nano</i> , 2019, 13, 9735-9780.	7.3	32
23	Mapping mesoscopic phase evolution during E-beam induced transformations via deep learning of atomically resolved images. <i>Npj Computational Materials</i> , 2018, 4, .	3.5	31
24	Exploration of Electrochemical Reactions at Organic-Inorganic Halide Perovskite Interfaces via Machine Learning in In Situ Time-of-Flight Secondary Ion Mass Spectrometry. <i>Advanced Functional Materials</i> , 2020, 30, 2001995.	7.8	30
25	Hypothesis Learning in Automated Experiment: Application to Combinatorial Materials Libraries. <i>Advanced Materials</i> , 2022, 34, e2201345.	11.1	30
26	Data mining for better material synthesis: The case of pulsed laser deposition of complex oxides. <i>Journal of Applied Physics</i> , 2018, 123, .	1.1	29
27	Off-the-shelf deep learning is not enough, and requires parsimony, Bayesianity, and causality. <i>Npj Computational Materials</i> , 2021, 7, .	3.5	28
28	Ensemble learning-iterative training machine learning for uncertainty quantification and automated experiment in atom-resolved microscopy. <i>Npj Computational Materials</i> , 2021, 7, .	3.5	26
29	Atomic Mechanisms for the Si Atom Dynamics in Graphene: Chemical Transformations at the Edge and in the Bulk. <i>Advanced Functional Materials</i> , 2019, 29, 1904480.	7.8	25
30	Lab on a beam-Big data and artificial intelligence in scanning transmission electron microscopy. <i>MRS Bulletin</i> , 2019, 44, 565-575.	1.7	24
31	Learning from Imperfections: Predicting Structure and Thermodynamics from Atomic Imaging of Fluctuations. <i>ACS Nano</i> , 2019, 13, 718-727.	7.3	24
32	Autonomous Experiments in Scanning Probe Microscopy and Spectroscopy: Choosing Where to Explore Polarization Dynamics in Ferroelectrics. <i>ACS Nano</i> , 2021, 15, 11253-11262.	7.3	23
33	Automated Experiment in 4D-STEM: Exploring Emergent Physics and Structural Behaviors. <i>ACS Nano</i> , 2022, 16, 7605-7614.	7.3	23
34	Toward Decoding the Relationship between Domain Structure and Functionality in Ferroelectrics via Hidden Latent Variables. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 1693-1703.	4.0	22
35	Deep data mining in a real space: separation of intertwined electronic responses in a lightly doped BaFe_2As_2 . <i>Nanotechnology</i> , 2016, 27, 475706.	1.3	21
36	Causal analysis of competing atomistic mechanisms in ferroelectric materials from high-resolution scanning transmission electron microscopy data. <i>Npj Computational Materials</i> , 2020, 6, .	3.5	21

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37	Building ferroelectric from the bottom up: The machine learning analysis of the atomic-scale ferroelectric distortions. <i>Applied Physics Letters</i> , 2019, 115, .	1.5	20
38	Imaging mechanism for hyperspectral scanning probe microscopy via Gaussian process modelling. <i>Npj Computational Materials</i> , 2020, 6, .	3.5	19
39	Disentangling Rotational Dynamics and Ordering Transitions in a System of Self-Organizing Protein Nanorods via Rotationally Invariant Latent Representations. <i>ACS Nano</i> , 2021, 15, 6471-6480.	7.3	19
40	Data mining graphene: correlative analysis of structure and electronic degrees of freedom in graphenic monolayers with defects. <i>Nanotechnology</i> , 2016, 27, 495703.	1.3	18
41	167-PFlops Deep Learning for Electron Microscopy: From Learning Physics to Atomic Manipulation. , 2018, , .		18
42	Exploring physics of ferroelectric domain walls via Bayesian analysis of atomically resolved STEM data. <i>Nature Communications</i> , 2020, 11, 6361.	5.8	17
43	Quantifying the Dynamics of Protein Self-Organization Using Deep Learning Analysis of Atomic Force Microscopy Data. <i>Nano Letters</i> , 2021, 21, 158-165.	4.5	17
44	Predictability of Localized Plasmonic Responses in Nanoparticle Assemblies. <i>Small</i> , 2021, 17, e2100181.	5.2	17
45	Disentangling Ferroelectric Wall Dynamics and Identification of Pinning Mechanisms via Deep Learning. <i>Advanced Materials</i> , 2021, 33, e2103680.	11.1	17
46	Deep data analytics for genetic engineering of diatoms linking genotype to phenotype via machine learning. <i>Npj Computational Materials</i> , 2019, 5, .	3.5	16
47	Computational scanning tunneling microscope image database. <i>Scientific Data</i> , 2021, 8, 57.	2.4	15
48	Probing atomic-scale symmetry breaking by rotationally invariant machine learning of multidimensional electron scattering. <i>Npj Computational Materials</i> , 2021, 7, .	3.5	15
49	Multi-objective Bayesian optimization of ferroelectric materials with interfacial control for memory and energy storage applications. <i>Journal of Applied Physics</i> , 2021, 130, .	1.1	15
50	Deep Bayesian local crystallography. <i>Npj Computational Materials</i> , 2021, 7, .	3.5	15
51	Identifying local structural states in atomic imaging by computer vision. <i>Advanced Structural and Chemical Imaging</i> , 2016, 2, 14.	4.0	14
52	Disentangling ferroelectric domain wall geometries and pathways in dynamic piezoresponse force microscopy via unsupervised machine learning. <i>Nanotechnology</i> , 2022, 33, 055707.	1.3	14
53	Physics makes the difference: Bayesian optimization and active learning via augmented Gaussian process. <i>Machine Learning: Science and Technology</i> , 2022, 3, 015003.	2.4	14
54	Separating Physically Distinct Mechanisms in Complex Infrared Plasmonic Nanostructures via Machine Learning Enhanced Electron Energy Loss Spectroscopy. <i>Advanced Optical Materials</i> , 2021, 9, 2001808.	3.6	13

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55	Revealing the Chemical Bonding in Adatom Arrays via Machine Learning of Hyperspectral Scanning Tunneling Spectroscopy Data. ACS Nano, 2021, 15, 11806-11816.	7.3	13
56	Chemically induced topological zero mode at graphene armchair edges. Physical Chemistry Chemical Physics, 2017, 19, 5145-5154.	1.3	12
57	Exploring Causal Physical Mechanisms via Non-Gaussian Linear Models and Deep Kernel Learning: Applications for Ferroelectric Domain Structures. ACS Nano, 2022, 16, 1250-1259.	7.3	12
58	Towards automating structural discovery in scanning transmission electron microscopy [*]. Machine Learning: Science and Technology, 2022, 3, 015024.	2.4	11
59	Tracking atomic structure evolution during directed electron beam induced Si-atom motion in graphene via deep machine learning. Nanotechnology, 2021, 32, 035703.	1.3	10
60	Bridging microscopy with molecular dynamics and quantum simulations: an atomAI based pipeline. Npj Computational Materials, 2022, 8, .	3.5	10
61	Guided search for desired functional responses via Bayesian optimization of generative model: Hysteresis loop shape engineering in ferroelectrics. Journal of Applied Physics, 2020, 128, .	1.1	9
62	Analysis of citation networks as a new tool for scientific research. MRS Bulletin, 2016, 41, 1009-1016.	1.7	8
63	Bayesian Learning of Adatom Interactions from Atomically Resolved Imaging Data. ACS Nano, 2021, 15, 9649-9657.	7.3	8
64	Exploration of lattice Hamiltonians for functional and structural discovery via Gaussian process-based exploration"exploitation. Journal of Applied Physics, 2020, 128, 164304.	1.1	8
65	Predictability as a probe of manifest and latent physics: The case of atomic scale structural, chemical, and polarization behaviors in multiferroic Sm-doped BiFeO3. Applied Physics Reviews, 2021, 8, .	5.5	7
66	Investigating phase transitions from local crystallographic analysis based on statistical learning of atomic environments in 2D MoS2-ReS2. Applied Physics Reviews, 2021, 8, 011409.	5.5	7
67	Latent Mechanisms of Polarization Switching from In Situ Electron Microscopy Observations. Advanced Functional Materials, 2022, 32, .	7.8	7
68	Super-resolution and signal separation in contact Kelvin probe force microscopy of electrochemically active ferroelectric materials. Journal of Applied Physics, 2020, 128, 055101.	1.1	6
69	Gaussian process analysis of electron energy loss spectroscopy data: multivariate reconstruction and kernel control. Npj Computational Materials, 2021, 7, .	3.5	6
70	Identification and correction of temporal and spatial distortions in scanning transmission electron microscopy. Ultramicroscopy, 2021, 229, 113337.	0.8	6
71	Deep learning of interface structures from simulated 4D STEM data: cation intermixing vs. roughening ^{&sup>—} </sup>. Machine Learning: Science and Technology, 2020, 1, 04LT01.	2.4	6
72	Deep Learning for Atomically Resolved Imaging. Microscopy and Microanalysis, 2018, 24, 60-61.	0.2	5

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73	Deep Convolutional Neural Networks for Symmetry Detection. <i>Microscopy and Microanalysis</i> , 2018, 24, 112-113.	0.2	5
74	Probing potential energy landscapes via electron-beam-induced single atom dynamics. <i>Acta Materialia</i> , 2021, 203, 116508.	3.8	5
75	Deep learning ferroelectric polarization distributions from STEM data via with and without atom finding. <i>Npj Computational Materials</i> , 2021, 7, .	3.5	5
76	Decoding the shift-invariant data: applications for band-excitation scanning probe microscopy [*]. <i>Machine Learning: Science and Technology</i> , 2021, 2, 045028.	2.4	5
77	Probing polarization dynamics at specific domain configurations: Computer-vision based automated experiment in piezoresponse force microscopy. <i>Applied Physics Letters</i> , 2021, 119, .	1.5	5
78	Reconstruction of effective potential from statistical analysis of dynamic trajectories. <i>AIP Advances</i> , 2020, 10, .	0.6	4
79	Alignment of Au nanorods along <i>de novo</i> designed protein nanofibers studied with automated image analysis. <i>Soft Matter</i> , 2021, 17, 6109-6115.	1.2	4
80	Exploring electron beam induced atomic assembly via reinforcement learning in a molecular dynamics environment. <i>Nanotechnology</i> , 2021, , .	1.3	4
81	Deep Data Analytics in Structural and Functional Imaging of Nanoscale Materials. <i>Springer Series in Materials Science</i> , 2018, , 103-128.	0.4	3
82	Statistical Physics-based Framework and Bayesian Inference for Model Selection and Uncertainty Quantification. <i>Microscopy and Microanalysis</i> , 2019, 25, 130-131.	0.2	3
83	Exploring Responses of Contact Kelvin Probe Force Microscopy in Triple-Cation Double-Halide Perovskites. <i>Journal of Physical Chemistry C</i> , 2021, 125, 12355-12365.	1.5	3
84	AtomAI: Open-source software for applications of deep learning to microscopy data. <i>Microscopy and Microanalysis</i> , 2021, 27, 3000-3002.	0.2	3
85	Beyond NMF: Advanced Signal Processing and Machine Learning Methodologies for Hyperspectral Analysis in EELS. <i>Microscopy and Microanalysis</i> , 2021, 27, 322-324.	0.2	3
86	Reconstruction of the interatomic forces from dynamic scanning transmission electron microscopy data. <i>Journal of Applied Physics</i> , 2020, 127, 224301.	1.1	2
87	Building an edge computing infrastructure for rapid multi-dimensional electron microscopy. <i>Microscopy and Microanalysis</i> , 2021, 27, 56-57.	0.2	2
88	Denoising STEM Electron Energy Loss Spectra using Convolutional Autoencoders. <i>Microscopy and Microanalysis</i> , 2021, 27, 1180-1182.	0.2	2
89	Reconstruction and uncertainty quantification of lattice Hamiltonian model parameters from observations of microscopic degrees of freedom. <i>Journal of Applied Physics</i> , 2020, 128, 214103.	1.1	2
90	Nanoscale interlayer defects in iron arsenides. <i>Journal of Solid State Chemistry</i> , 2019, 277, 422-426.	1.4	1

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91	Thermodynamics of order and randomness in dopant distributions inferred from atomically resolved imaging. Npj Computational Materials, 2021, 7, .	3.5	1
92	Automated Experiment in SPM: Bayesian Optimization for efficient searching of parameter space to maximize functional response. Microscopy and Microanalysis, 2021, 27, 470-471.	0.2	1
93	Probing atomic-scale symmetry breaking by rotationally invariant machine learning of 4D-STEM Data.. Microscopy and Microanalysis, 2021, 27, 2200-2201.	0.2	1
94	Bayesian Inference for Materials Physics from STEM Data: The Probability Distribution of Physical Parameters from Ferroelectric Domain Wall Observations. Microscopy and Microanalysis, 2021, 27, 1212-1214.	0.2	1
95	Deep Data Mining in a Real Space: Application to Scanning Probe Microscopy Studies on a "Parent" State of a High Temperature Superconductor. Microscopy and Microanalysis, 2016, 22, 1418-1419.	0.2	0
96	Phase determination from atomically resolved images: physics-constrained deep data analysis through an unmixing approach. Microscopy and Microanalysis, 2016, 22, 1452-1453.	0.2	0
97	Atomic Level Structure-Property Relationship in a Spin-Orbit Mott insulator: Scanning Transmission Electron and Scanning Tunneling Microscopy Studies. Microscopy and Microanalysis, 2016, 22, 908-909.	0.2	0
98	Leveraging Single Atom Dynamics to Measure the Electron-Beam-Induced Force and Atomic Potentials. Microscopy and Microanalysis, 2018, 24, 96-97.	0.2	0
99	Machine Learning for the Dynamic Scanning Transmission Electron Microscopy Experiment on Solid State Transformations. Microscopy and Microanalysis, 2018, 24, 1600-1601.	0.2	0
100	FerroNet: Machine Learning Flow for Analysis of Ferroelectric and Ferroelastic Materials. Microscopy and Microanalysis, 2019, 25, 170-171.	0.2	0
101	Towards Atomic Scale Quantum Structure Fabrication in 2D Materials. Microscopy and Microanalysis, 2019, 25, 940-941.	0.2	0
102	Causal Learning from Structural and Spectral Electron Microscopy Data. Microscopy and Microanalysis, 2020, 26, 6-6.	0.2	0
103	Mapping the Distortion Function via Multivariate Analysis of Atomically Resolved Images. Microscopy and Microanalysis, 2020, 26, 2134-2135.	0.2	0
104	Towards Automating Structural Discovery in Scanning Transmission Electron Microscopy. Microscopy and Microanalysis, 2021, 27, 2770-2772.	0.2	0
105	Deep Learning-Based Workflow for Analyzing Helium Bubbles in Transmission Electron Microscopy Images. Microscopy and Microanalysis, 2021, 27, 2132-2133.	0.2	0
106	Causal Analysis of Parameterized Atomic HAADF-STEM Across a Doped Ferroelectric Phase Boundary. Microscopy and Microanalysis, 2021, 27, 2762-2764.	0.2	0
107	Direct mapping of polarization fields from STEM images: A Deep Learning based exploration of ferroelectrics. Microscopy and Microanalysis, 2021, 27, 2990-2992.	0.2	0
108	Predicting local plasmon resonances and geometries using autoencoder networks in complex nanoparticle assemblies. Microscopy and Microanalysis, 2021, 27, 2766-2768.	0.2	0

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109	Deep Machine Learning in Electron and Scanning Probe Microscopy. , 2020, , 363-395.		0
110	Big and Deep Data Methods in Scanning Probe Microscopy and Spectroscopy. , 2020, , 301-362.		0
111	Strain-Induced asymmetry and on-site dynamics of silicon defects in graphene. Carbon Trends, 2022, 9, 100189.	1.4	0