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List of Publications by Year in Descending Order

104 papers	1,232 citations	18 h-index	32 g-index
116 ext. papers	1,744 ext. citations	8.2 avg, IF	4.92 L-index

#	Paper	IF	Citations
104	Physics makes the difference: Bayesian optimization and active learning via augmented Gaussian process. *Machine Learning: Science and Technology*, **2022**, 3, 015022	5.1	2
103	Machine learning in scanning transmission electron microscopy. *Nature Reviews Methods Primers*, **2022**, 2,		5
102	Hypothesis learning in automated experiment: application to combinatorial materials libraries.. *Advanced Materials*, **2022**, e2201345	24	3
101	Automated Experiment in 4D-STEM: Exploring Emergent Physics and Structural Behaviors.. *ACS Nano*, **2022**,	16.7	3
100	Tracking atomic structure evolution during directed electron beam induced Si-atom motion in graphene via deep machine learning. *Nanotechnology*, **2021**, 32, 035703	3.4	4
99	Multi-objective Bayesian optimization of ferroelectric materials with interfacial control for memory and energy storage applications. *Journal of Applied Physics*, **2021**, 130, 204102	2.5	0
98	High-Throughput Study of Antisolvents on the Stability of Multicomponent Metal Halide Perovskites through Robotics-Based Synthesis and Machine Learning Approaches. *Journal of the American Chemical Society*, **2021**, 143, 19945-19955	16.4	4
97	Deep Bayesian local crystallography. *Npj Computational Materials*, **2021**, 7,	10.9	5
96	Disentangling ferroelectric domain wall geometries and pathways in dynamic piezoresponse force microscopy via unsupervised machine learning. *Nanotechnology*, **2021**, 33,	3.4	5
95	Machine learning for high-throughput experimental exploration of metal halide perovskites. *Joule*, **2021**,	27.8	7
94	Thermodynamics of order and randomness in dopant distributions inferred from atomically resolved imaging. *Npj Computational Materials*, **2021**, 7,	10.9	1
93	Investigating phase transitions from local crystallographic analysis based on statistical learning of atomic environments in 2D MoS2-ReS2. *Applied Physics Reviews*, **2021**, 8, 011409	17.3	1
92	Exploring order parameters and dynamic processes in disordered systems via variational autoencoders. *Science Advances*, **2021**, 7,	14.3	11
91	Disentangling Rotational Dynamics and Ordering Transitions in a System of Self-Organizing Protein Nanorods Rotationally Invariant Latent Representations. *ACS Nano*, **2021**, 15, 6471-6480	16.7	7
90	Separating Physically Distinct Mechanisms in Complex Infrared Plasmonic Nanostructures via Machine Learning Enhanced Electron Energy Loss Spectroscopy. *Advanced Optical Materials*, **2021**, 9, 2001808	8.1	7
89	Predictability of Localized Plasmonic Responses in Nanoparticle Assemblies. *Small*, **2021**, 17, e2100181	11	7
88	Probing atomic-scale symmetry breaking by rotationally invariant machine learning of multidimensional electron scattering. *Npj Computational Materials*, **2021**, 7,	10.9	6

87	Exploring Responses of Contact Kelvin Probe Force Microscopy in Triple-Cation Double-Halide Perovskites. *Journal of Physical Chemistry C*, **2021**, 125, 12355-12365	3.8	0
86	Revealing the Chemical Bonding in Adatom Arrays via Machine Learning of Hyperspectral Scanning Tunneling Spectroscopy Data. *ACS Nano*, **2021**,	16.7	4
85	Bayesian Learning of Adatom Interactions from Atomically Resolved Imaging Data. *ACS Nano*, **2021**, 15, 9649-9657	16.7	2
84	Automated Experiment in SPM: Bayesian Optimization for efficient searching of parameter space to maximize functional response. *Microscopy and Microanalysis*, **2021**, 27, 470-471	0.5	1
83	Building an edge computing infrastructure for rapid multi-dimensional electron microscopy. *Microscopy and Microanalysis*, **2021**, 27, 56-57	0.5	0
82	Towards Automating Structural Discovery in Scanning Transmission Electron Microscopy. *Microscopy and Microanalysis*, **2021**, 27, 2770-2772	0.5	
81	Probing atomic-scale symmetry breaking by rotationally invariant machine learning of 4D-STEM Data.. *Microscopy and Microanalysis*, **2021**, 27, 2200-2201	0.5	0
80	Ensemble learning-iterative training machine learning for uncertainty quantification and automated experiment in atom-resolved microscopy. *Npj Computational Materials*, **2021**, 7,	10.9	4
79	Autonomous Experiments in Scanning Probe Microscopy and Spectroscopy: Choosing Where to Explore Polarization Dynamics in Ferroelectrics. *ACS Nano*, **2021**,	16.7	8
78	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	0.5	
77	AtomAI: Open-source software for applications of deep learning to microscopy data. *Microscopy and Microanalysis*, **2021**, 27, 3000-3002	0.5	1
76	Automated and Autonomous Experiments in Electron and Scanning Probe Microscopy. *ACS Nano*, **2021**,	16.7	11
75	Probing potential energy landscapes via electron-beam-induced single atom dynamics. *Acta Materialia*, **2021**, 203, 116508	8.4	2
74	Quantifying the Dynamics of Protein Self-Organization Using Deep Learning Analysis of Atomic Force Microscopy Data. *Nano Letters*, **2021**, 21, 158-165	11.5	7
73	Alignment of Au nanorods along designed protein nanofibers studied with automated image analysis. *Soft Matter*, **2021**, 17, 6109-6115	3.6	3
72	Toward Decoding the Relationship between Domain Structure and Functionality in Ferroelectrics via Hidden Latent Variables. *ACS Applied Materials & Interfaces*, **2021**, 13, 1693-1703	9.5	14
71	Off-the-shelf deep learning is not enough, and requires parsimony, Bayesianity, and causality. *Npj Computational Materials*, **2021**, 7,	10.9	4
70	Computational scanning tunneling microscope image database. *Scientific Data*, **2021**, 8, 57	8.2	4

69	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, 011403	17.3	2
68	Deep Learning-Based Workflow for Analyzing Helium Bubbles in Transmission Electron Microscopy Images. *Microscopy and Microanalysis*, **2021**, 27, 2132-2133	0.5	
67	Causal Analysis of Parameterized Atomic HAADF-STEM Across a Doped Ferroelectric Phase Boundary. *Microscopy and Microanalysis*, **2021**, 27, 2762-2764	0.5	
66	Direct mapping of polarization fields from STEM images: A Deep Learning based exploration of ferroelectrics. *Microscopy and Microanalysis*, **2021**, 27, 2990-2992	0.5	
65	Denoising STEM Electron Energy Loss Spectra using Convolutional Autoencoders. *Microscopy and Microanalysis*, **2021**, 27, 1180-1182	0.5	0
64	Predicting local plasmon resonances and geometries using autoencoder networks in complex nanoparticle assemblies. *Microscopy and Microanalysis*, **2021**, 27, 2766-2768	0.5	
63	Beyond NMF: Advanced Signal Processing and Machine Learning Methodologies for Hyperspectral Analysis in EELS. *Microscopy and Microanalysis*, **2021**, 27, 322-324	0.5	0
62	Deep learning ferroelectric polarization distributions from STEM data via with and without atom finding. *Npj Computational Materials*, **2021**, 7,	10.9	1
61	Disentangling Ferroelectric Wall Dynamics and Identification of Pinning Mechanisms via Deep Learning. *Advanced Materials*, **2021**, 33, e2103680	24	7
60	Gaussian process analysis of electron energy loss spectroscopy data: multivariate reconstruction and kernel control. *Npj Computational Materials*, **2021**, 7,	10.9	2
59	Probing polarization dynamics at specific domain configurations: Computer-vision based automated experiment in piezoresponse force microscopy. *Applied Physics Letters*, **2021**, 119, 132902	3.4	3
58	Identification and correction of temporal and spatial distortions in scanning transmission electron microscopy. *Ultramicroscopy*, **2021**, 229, 113337	3.1	2
57	Mapping the Distortion Function via Multivariate Analysis of Atomically Resolved Images. *Microscopy and Microanalysis*, **2020**, 26, 2134-2135	0.5	
56	Reconstruction of the interatomic forces from dynamic scanning transmission electron microscopy data. *Journal of Applied Physics*, **2020**, 127, 224301	2.5	1
55	Guided search for desired functional responses via Bayesian optimization of generative model: Hysteresis loop shape engineering in ferroelectrics. *Journal of Applied Physics*, **2020**, 128, 024102	2.5	4
54	Reconstruction of effective potential from statistical analysis of dynamic trajectories. *AIP Advances*, **2020**, 10, 065034	1.5	2
53	Exploration of Electrochemical Reactions at Organic-Inorganic Halide Perovskite Interfaces via Machine Learning in In Situ Time-of-Flight Secondary Ion Mass Spectrometry. *Advanced Functional Materials*, **2020**, 30, 2001995	15.6	15
52	Imaging mechanism for hyperspectral scanning probe microscopy via Gaussian process modelling. *Npj Computational Materials*, **2020**, 6,	10.9	9

51	Big and Deep Data Methods in Scanning Probe Microscopy and Spectroscopy **2020**, 301-362		
50	Deep Machine Learning in Electron and Scanning Probe Microscopy **2020**, 363-395		
49	Exploration of lattice Hamiltonians for functional and structural discovery via Gaussian process-based exploration-exploitation. *Journal of Applied Physics*, **2020**, 128, 164304	2.5	4
48	Reconstruction and uncertainty quantification of lattice Hamiltonian model parameters from observations of microscopic degrees of freedom. *Journal of Applied Physics*, **2020**, 128, 214103	2.5	1
47	Deep learning of interface structures from simulated 4D STEM data: cation intermixing vs. roughening. *Machine Learning: Science and Technology*, **2020**, 1, 04LT01	5.1	3
46	Chemical Robotics Enabled Exploration of Stability in Multicomponent Lead Halide Perovskites via Machine Learning. *ACS Energy Letters*, **2020**, 5, 3426-3436	20.1	24
45	Causal Learning from Structural and Spectral Electron Microscopy Data. *Microscopy and Microanalysis*, **2020**, 26, 6-6	0.5	
44	Fast Scanning Probe Microscopy via Machine Learning: Non-Rectangular Scans with Compressed Sensing and Gaussian Process Optimization. *Small*, **2020**, 16, e2002878	11	19
43	Super-resolution and signal separation in contact Kelvin probe force microscopy of electrochemically active ferroelectric materials. *Journal of Applied Physics*, **2020**, 128, 055101	2.5	3
42	Causal analysis of competing atomistic mechanisms in ferroelectric materials from high-resolution scanning transmission electron microscopy data. *Npj Computational Materials*, **2020**, 6,	10.9	10
41	Exploring physics of ferroelectric domain walls via Bayesian analysis of atomically resolved STEM data. *Nature Communications*, **2020**, 11, 6361	17.4	7
40	FerroNet: Machine Learning Flow for Analysis of Ferroelectric and Ferroelastic Materials. *Microscopy and Microanalysis*, **2019**, 25, 170-171	0.5	
39	Building and exploring libraries of atomic defects in graphene: Scanning transmission electron and scanning tunneling microscopy study. *Science Advances*, **2019**, 5, eaaw8989	14.3	41
38	Towards Atomic Scale Quantum Structure Fabrication in 2D Materials. *Microscopy and Microanalysis*, **2019**, 25, 940-941	0.5	
37	Deep learning analysis of defect and phase evolution during electron beam-induced transformations in WS2. *Npj Computational Materials*, **2019**, 5,	10.9	74
36	Atom-by-atom fabrication with electron beams. *Nature Reviews Materials*, **2019**, 4, 497-507	73.3	42
35	Deep data analytics for genetic engineering of diatoms linking genotype to phenotype via machine learning. *Npj Computational Materials*, **2019**, 5,	10.9	9
34	Toward Electrochemical Studies on the Nanometer and Atomic Scales: Progress, Challenges, and Opportunities. *ACS Nano*, **2019**, 13, 9735-9780	16.7	18

33	Building ferroelectric from the bottom up: The machine learning analysis of the atomic-scale ferroelectric distortions. *Applied Physics Letters*, **2019**, 115, 052902	3.4	13
32	Statistical Physics-based Framework and Bayesian Inference for Model Selection and Uncertainty Quantification. *Microscopy and Microanalysis*, **2019**, 25, 130-131	0.5	2
31	Lab on a beamBig data and artificial intelligence in scanning transmission electron microscopy. *MRS Bulletin*, **2019**, 44, 565-575	3.2	15
30	Materials Science in the AI age: high-throughput library generation, machine learning and a pathway from correlations to the underpinning physics. *MRS Communications*, **2019**, 9, 821	2.7	56
29	Nanoscale interlayer defects in iron arsenides. *Journal of Solid State Chemistry*, **2019**, 277, 422-426	3.3	1
28	Atomic Mechanisms for the Si Atom Dynamics in Graphene: Chemical Transformations at the Edge and in the Bulk. *Advanced Functional Materials*, **2019**, 29, 1904480	15.6	17
27	Learning from Imperfections: Predicting Structure and Thermodynamics from Atomic Imaging of Fluctuations. *ACS Nano*, **2019**, 13, 718-727	16.7	19
26	Data mining for better material synthesis: The case of pulsed laser deposition of complex oxides. *Journal of Applied Physics*, **2018**, 123, 115303	2.5	18
25	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	3.9	27
24	Deep Learning for Atomically Resolved Imaging. *Microscopy and Microanalysis*, **2018**, 24, 60-61	0.5	2
23	Leveraging Single Atom Dynamics to Measure the Electron-Beam-Induced Force and Atomic Potentials. *Microscopy and Microanalysis*, **2018**, 24, 96-97	0.5	
22	Deep Convolutional Neural Networks for Symmetry Detection. *Microscopy and Microanalysis*, **2018**, 24, 112-113	0.5	2
21	Machine Learning for the Dynamic Scanning Transmission Electron Microscopy Experiment on Solid State Transformations. *Microscopy and Microanalysis*, **2018**, 24, 1600-1601	0.5	
20	167-PFlops Deep Learning for Electron Microscopy: From Learning Physics to Atomic Manipulation **2018**,		15
19	Deep Data Analytics in Structural and Functional Imaging of Nanoscale Materials. *Springer Series in Materials Science*, **2018**, 103-128	0.9	3
18	Mapping mesoscopic phase evolution during E-beam induced transformations via deep learning of atomically resolved images. *Npj Computational Materials*, **2018**, 4,	10.9	24
17	Chemically induced topological zero mode at graphene armchair edges. *Physical Chemistry Chemical Physics*, **2017**, 19, 5145-5154	3.6	11
16	Identifying local structural states in atomic imaging by computer vision. *Advanced Structural and Chemical Imaging*, **2017**, 2, 14	3.9	9

15	Learning surface molecular structures via machine vision. *Npj Computational Materials*, **2017**, 3,	10.9	60
14	Deep Learning of Atomically Resolved Scanning Transmission Electron Microscopy Images: Chemical Identification and Tracking Local Transformations. *ACS Nano*, **2017**, 11, 12742-12752	16.7	183
13	Bowl Inversion and Electronic Switching of Buckybowls on Gold. *Journal of the American Chemical Society*, **2016**, 138, 12142-9	16.4	38
12	Data mining graphene: correlative analysis of structure and electronic degrees of freedom in graphenic monolayers with defects. *Nanotechnology*, **2016**, 27, 495703	3.4	13
11	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	0.5	
10	Phase determination from atomically resolved images: physics-constrained deep data analysis through an unmixing approach. *Microscopy and Microanalysis*, **2016**, 22, 1452-1453	0.5	
9	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	0.5	
8	Deep data mining in a real space: separation of intertwined electronic responses in a lightly doped BaFeAs. *Nanotechnology*, **2016**, 27, 475706	3.4	20
7	Analysis of citation networks as a new tool for scientific research. *MRS Bulletin*, **2016**, 41, 1009-1016	3.2	6
6	Atomic-scale observation of structural and electronic orders in the layered compound α-RuCl. *Nature Communications*, **2016**, 7, 13774	17.4	50
5	Phases and Interfaces from Real Space Atomically Resolved Data: Physics-Based Deep Data Image Analysis. *Nano Letters*, **2016**, 16, 5574-81	11.5	26
4	Role of edge geometry and chemistry in the electronic properties of graphene nanostructures. *Faraday Discussions*, **2014**, 173, 173-99	3.6	54
3	Direct imaging of monovacancy-hydrogen complexes in a single graphitic layer. *Physical Review B*, **2014**, 89,	3.3	43
2	Visualization of electronic states on atomically smooth graphitic edges with different types of hydrogen termination. *Physical Review B*, **2013**, 87,	3.3	41
1	Latent Mechanisms of Polarization Switching from In Situ Electron Microscopy Observations. *Advanced Functional Materials*,2100271	15.6	1