Kipton Barros

List of Publications by Year in descending order

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42 papers	2,280 citations	279798 23 h-index	265206 42 g-index
45 all docs	45 docs citations	45 times ranked	2130 citing authors

#	Article	IF	Citations
1	Machine learning of consistent thermodynamic models using automatic differentiation. Physical Review E, 2022, 105, 045301.	2.1	7
2	Dynamical tuning of the chemical potential to achieve a target particle number in grand canonical Monte Carlo simulations. Physical Review E, 2022, 105, 045311.	2.1	6
3	Fast and scalable quantum Monte Carlo simulations of electron-phonon models. Physical Review E, 2022, 105, .	2.1	8
4	Deep learning of dynamically responsive chemical Hamiltonians with semiempirical quantum mechanics. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	7.1	19
5	Automated discovery of a robust interatomic potential for aluminum. Nature Communications, 2021, 12, 1257.	12.8	47
6	Machine learned HÃ¼ckel theory: Interfacing physics and deep neural networks. Journal of Chemical Physics, 2021, 154, 244108.	3.0	25
7	The Rise of Neural Networks for Materials and Chemical Dynamics. Journal of Physical Chemistry Letters, 2021, 12, 6227-6243.	4.6	39
8	Predicting phosphorescence energies and inferring wavefunction localization with machine learning. Chemical Science, 2021, 12, 10207-10217.	7.4	14
9	Phase diagram of a spin-ice Kondo lattice model in a breathing pyrochlore lattice. Physical Review B, 2020, 102, .	3.2	2
10	Machine learning approaches for structural and thermodynamic properties of a Lennard-Jones fluid. Journal of Chemical Physics, 2020, 153, 104502.	3.0	22
11	Langevin simulations of the half-filled cubic Holstein model. Physical Review B, 2020, 102, .	3.2	18
12	The ANI-1ccx and ANI-1x data sets, coupled-cluster and density functional theory properties for molecules. Scientific Data, 2020, 7, 134.	5.3	104
13	Ex Machina Determination of Structural Correlation Functions. Journal of Physical Chemistry Letters, 2020, 11, 4372-4378.	4.6	7
14	Extending the Applicability of the ANI Deep Learning Molecular Potential to Sulfur and Halogens. Journal of Chemical Theory and Computation, 2020, 16, 4192-4202.	5.3	160
15	Approaching coupled cluster accuracy with a general-purpose neural network potential through transfer learning. Nature Communications, 2019, 10, 2903.	12.8	399
16	Nonequilibrium dynamics of superconductivity in the attractive Hubbard model. Physical Review B, 2019, 99, .	3.2	3
17	Machine learning for molecular dynamics with strongly correlated electrons. Physical Review B, 2019, 99, .	3.2	20
18	Anomalous magnetoresistance due to longitudinal spin fluctuations in a Jeffâ€‰=â€‰1/2 Mott semiconductor. Nature Communications, 2019, 10, 5301.	12.8	12

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19	Hierarchical modeling of molecular energies using a deep neural network. Journal of Chemical Physics, 2018, 148, 241715.	3.0	221
20	Semiclassical dynamics of spin density waves. Physical Review B, 2018, 97, .	3.2	27
21	Gradient-based stochastic estimation of the density matrix. Journal of Chemical Physics, 2018, 148, .	3.0	24
22	Earthquake Catalogâ€Based Machine Learning Identification of Laboratory Fault States and the Effects of Magnitude of Completeness. Geophysical Research Letters, 2018, 45, 13,269.	4.0	39
23	Transferable Dynamic Molecular Charge Assignment Using Deep Neural Networks. Journal of Chemical Theory and Computation, 2018, 14, 4687-4698.	5.3	81
24	Discovering a Transferable Charge Assignment Model Using Machine Learning. Journal of Physical Chemistry Letters, 2018, 9, 4495-4501.	4.6	88
25	Learning molecular energies using localized graph kernels. Journal of Chemical Physics, 2017, 146, 114107.	3.0	48
26	Machine Learning Predicts Laboratory Earthquakes. Geophysical Research Letters, 2017, 44, 9276-9282.	4.0	272
27	Shape of magnetic domain walls formed by coupling to mobile charges. Physical Review B, 2017, 96, .	3.2	13
28	Automatized convergence of optoelectronic simulations using active machine learning. Applied Physics Letters, 2017, 111, .	3.3	9
29	Mott Transition in a Metallic Liquid: Gutzwiller Molecular Dynamics Simulations. Physical Review Letters, 2017, 118, 226401.	7.8	10
30	Vortex Crystals with Chiral Stripes in Itinerant Magnets. Journal of the Physical Society of Japan, 2016, 85, 103703.	1.6	85
31	Optimisation of GaN LEDs and the reduction of efficiency droop using active machine learning. Scientific Reports, 2016, 6, 24862.	3.3	43
32	Resistivity Minimum in Highly Frustrated Itinerant Magnets. Physical Review Letters, 2016, 117, 206601.	7.8	33
33	Physics-based statistical learning approach to mesoscopic model selection. Physical Review E, 2015, 92, 053301.	2.1	6
34	Comparison of efficient techniques for the simulation of dielectric objects in electrolytes. Journal of Computational Physics, 2015, 291, 317-333.	3.8	23
35	Distributed Database Kriging for Adaptive Sampling (D2KAS). Computer Physics Communications, 2015, 192, 138-147.	7.5	23
36	Exotic magnetic orderings in the kagome Kondo-lattice model. Physical Review B, 2014, 90, .	3.2	52

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37	Dielectric Effects in the Self-Assembly of Binary Colloidal Aggregates. Physical Review Letters, 2014, 113, 017801.	7.8	100
38	Spatial adaptive sampling in multiscale simulation. Computer Physics Communications, 2014, 185, 1857-1864.	7.5	23
39	Magnetic-field-induced phases in anisotropic triangular antiferromagnets: Application to <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>CuCrO</mml:mi><mml:mn>2</mml:mn></mml:msub> Physical Review B, 2014, 89, .	3.2	15
40	Efficient and accurate simulation of dynamic dielectric objects. Journal of Chemical Physics, 2014, 140, 064903.	3.0	63
41	Efficient Langevin simulation of coupled classical fields and fermions. Physical Review B, 2013, 88, .	3.2	56
42	Liquid to solid nucleation via onion structure droplets. Journal of Chemical Physics, 2013, 139, 174505.	3.0	10