Yaolong Zhang

List of Publications by Year
in descending order

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		361045	525886
27	1,003	20	27
papers	citations	h-index	g-index

27	27	27	542
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	REANN: A PyTorch-based end-to-end multi-functional deep neural network package for molecular, reactive, and periodic systems. Journal of Chemical Physics, 2022, 156, 114801.	1.2	19
2	Accelerating atomistic simulations with piecewise machine-learned ab Initio potentials at a classical force field-like cost. Physical Chemistry Chemical Physics, 2021, 23, 1815-1821.	1.3	24
3	Searching Configurations in Uncertainty Space: Active Learning of High-Dimensional Neural Network Reactive Potentials. Journal of Chemical Theory and Computation, 2021, 17, 2691-2701.	2.3	39
4	A Machine-Learning Protocol for Ultraviolet Protein-Backbone Absorption Spectroscopy under Environmental Fluctuations. Journal of Physical Chemistry B, 2021, 125, 6171-6178.	1.2	13
5	Photoinduced Desorption Dynamics of CO from Pd(111): A Neural Network Approach. Journal of Chemical Theory and Computation, 2021, 17, 4648-4659.	2.3	15
6	Neural Network Representations for Studying <scp>Gasâ€Surface</scp> Reaction Dynamics: Beyond the <scp>Bornâ€Oppenheimer</scp> Static Surface Approximation^{â€}. Chinese Journal of Chemistry, 2021, 39, 2917-2930.	2.6	10
7	Towards bridging the structure gap in heterogeneous catalysis: the impact of defects in dissociative chemisorption of methane on Ir surfaces. Physical Chemistry Chemical Physics, 2021, 23, 4376-4385.	1.3	31
8	Determining the Effect of Hot Electron Dissipation on Molecular Scattering Experiments at Metal Surfaces. Jacs Au, 2021, 1, 164-173.	3.6	33
9	Physically Motivated Recursively Embedded Atom Neural Networks: Incorporating Local Completeness and Nonlocality. Physical Review Letters, 2021, 127, 156002.	2.9	32
10	Accurate Machine Learning Prediction of Protein Circular Dichroism Spectra with Embedded Density Descriptors. Jacs Au, 2021, 1, 2377-2384.	3.6	16
11	Symmetry-Adapted High Dimensional Neural Network Representation of Electronic Friction Tensor of Adsorbates on Metals. Journal of Physical Chemistry C, 2020, 124, 186-195.	1.5	45
12	Dynamics of H₂O Adsorption on Pt(110)-(1 Ã— 2) Based on a Neural Network Potential Energy Surface. Journal of Physical Chemistry C, 2020, 124, 23190-23199.	1.5	16
13	Efficient and Accurate Simulations of Vibrational and Electronic Spectra with Symmetry-Preserving Neural Network Models for Tensorial Properties. Journal of Physical Chemistry B, 2020, 124, 7284-7290.	1.2	51
14	Unified and transferable description of dynamics of H₂ dissociative adsorption on multiple copper surfaces via machine learning. Physical Chemistry Chemical Physics, 2020, 22, 13958-13964.	1.3	37
15	Efficient Construction of Excited-State Hessian Matrices with Machine Learning Accelerated Multilayer Energy-Based Fragment Method. Journal of Physical Chemistry A, 2020, 124, 5684-5695.	1.1	27
16	New Perspectives on CO₂â€“Pt(111) Interaction with a High-Dimensional Neural Network Potential Energy Surface. Journal of Physical Chemistry C, 2020, 124, 5174-5181.	1.5	37
17	Automatically growing global reactive neural network potential energy surfaces: A trajectory-free active learning strategy. Journal of Chemical Physics, 2020, 152, 154104.	1.2	40
18	Embedded Atom Neural Network Potentials: Efficient and Accurate Machine Learning with a Physically Inspired Representation. Journal of Physical Chemistry Letters, 2019, 10, 4962-4967.	2.1	157

#	Article	IF	Citations
19	Hot-electron effects during reactive scattering of H₂ from Ag(111): the interplay between mode-specific electronic friction and the potential energy landscape. Chemical Science, 2019, 10, 1089-1097.	3.7	35
20	Strong Vibrational Relaxation of NO Scattered from Au(111): Importance of the Adiabatic Potential Energy Surface. Journal of Physical Chemistry Letters, 2019, 10, 5969-5974.	2.1	35
21	Hot electron effects during reactive scattering of H₂ from Ag(111): assessing the sensitivity to initial conditions, coupling magnitude, and electronic temperature. Faraday Discussions, 2019, 214, 105-121.	1.6	15
22	Bridging the Gap between Direct Dynamics and Globally Accurate Reactive Potential Energy Surfaces Using Neural Networks. Journal of Physical Chemistry Letters, 2019, 10, 1185-1191.	2.1	65
23	Adiabatic and nonadiabatic energy dissipation during scattering of vibrationally excited CO from Au(111). Physical Review B, 2019, 100, .	1.1	23
24	Constructing High-Dimensional Neural Network Potential Energy Surfaces for Gasâ€“Surface Scattering and Reactions. Journal of Physical Chemistry C, 2018, 122, 1761-1769.	1.5	78
25	Vibrational control of selective bond cleavage in dissociative chemisorption of methanol on Cu(111). Nature Communications, 2018, 9, 4039.	5.8	30
26	Dissociative Chemisorption of O₂ on Al(111): Dynamics on a Correlated Wave-Function-Based Potential Energy Surface. Journal of Physical Chemistry Letters, 2018, 9, 3271-3277.	2.1	40
27	Dissociative chemisorption of methane on Ni(111) using a chemically accurate fifteen dimensional potential energy surface. Physical Chemistry Chemical Physics, 2017, 19, 30540-30550.	1.3	40