

Mohan Chen

List of Publications by Year in descending order

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50
papers

1,678
citations

377584

21
h-index

340414

39
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50
docs citations

50
times ranked

2204
citing authors

#	ARTICLE	IF	CITATIONS
1	Retention and recycling of deuterium in liquid lithium-tin slab studied by first-principles molecular dynamics. <i>Journal of Nuclear Materials</i> , 2021, 543, 152542.	1.3	2
2	86 PFLOPS Deep Potential Molecular Dynamics simulation of 100 million atoms with ab initio accuracy. <i>Computer Physics Communications</i> , 2021, 259, 107624.	3.0	100
3	Copper-doped beryllium and beryllium oxide interface: A first-principles study. <i>Journal of Nuclear Materials</i> , 2021, 545, 152733.	1.3	6
4	Thermal transport by electrons and ions in warm dense aluminum: A combined density functional theory and deep potential study. <i>Matter and Radiation at Extremes</i> , 2021, 6, .	1.5	13
5	Topological transformations in hyperuniform pentagonal two-dimensional materials induced by Stone-Wales defects. <i>Physical Review B</i> , 2021, 103, .	1.1	7
6	Editorial: Advances in Density Functional Theory and Beyond for Computational Chemistry. <i>Frontiers in Chemistry</i> , 2021, 9, 705762.	1.8	7
7	Modeling Liquid Water by Climbing up Jacob's Ladder in Density Functional Theory Facilitated by Using Deep Neural Network Potentials. <i>Journal of Physical Chemistry B</i> , 2021, 125, 11444-11456.	1.2	40
8	Stone-Wales defects preserve hyperuniformity in amorphous two-dimensional networks. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, .	3.3	28
9	Structure and dynamics of warm dense aluminum: a molecular dynamics study with density functional theory and deep potential. <i>Journal of Physics Condensed Matter</i> , 2020, 32, 144002.	0.7	21
10	Stabilization of Hydroxide Ions at the Interface of a Hydrophobic Monolayer on Water via Reduced Proton Transfer. <i>Physical Review Letters</i> , 2020, 125, 156803.	2.9	21
11	Deep neural network for the dielectric response of insulators. <i>Physical Review B</i> , 2020, 102, .	1.1	60
12	Electrical and thermal transport properties of medium-entropy Si Ge Sn alloys. <i>Acta Materialia</i> , 2020, 199, 443-452.	3.8	13
13	Disordered hyperuniformity in two-dimensional amorphous silica. <i>Science Advances</i> , 2020, 6, eaba0826.	4.7	35
14	Warm dense matter simulation via electron temperature dependent deep potential molecular dynamics. <i>Physics of Plasmas</i> , 2020, 27, .	0.7	19
15	Isotope effects in molecular structures and electronic properties of liquid water via deep potential molecular dynamics based on the SCAN functional. <i>Physical Review B</i> , 2020, 102, .	1.1	22
16	Pushing the Limit of Molecular Dynamics with Ab Initio Accuracy to 100 Million Atoms with Machine Learning. , 2020, , .		69
17	First-principles study of the infrared spectrum in liquid water from a systematically improved description of H-bond network. <i>Physical Review B</i> , 2019, 99, .	1.1	27
18	Structural, electronic, and dynamical properties of liquid water by <i>ab initio</i> molecular dynamics based on SCAN functional within the canonical ensemble. <i>Journal of Chemical Physics</i> , 2018, 148, 164505.	1.2	58

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19	Hydroxide diffuses slower than hydronium in water because its solvated structure inhibits correlated proton transfer. <i>Nature Chemistry</i> , 2018, 10, 413-419.	6.6	175
20	Signature of the hydrogen-bonded environment of liquid water in X-ray emission spectra from first-principles calculations. <i>Frontiers of Physics</i> , 2018, 13, 1.	2.4	3
21	Electron-Hole Theory of the Effect of Quantum Nuclei on the X-Ray Absorption Spectra of Liquid Water. <i>Physical Review Letters</i> , 2018, 121, 137401.	2.9	35
22	Finite-temperature infrared and Raman spectra of high-pressure hydrogen from first-principles molecular dynamics. <i>Physical Review B</i> , 2018, 98, .	1.1	14
23	Orbital-free density functional theory simulation of collective dynamics coupling in liquid Sn. <i>Journal of Chemical Physics</i> , 2018, 149, 094504.	1.2	16
24	Orbital-free density functional theory characterization of the Mg_2Al interface. <i>Journal of Chemical Physics</i> , 2018, 149, 094504.	0.9	3
25	Potential Functional Embedding Theory at the Correlated Wave Function Level. 1. Mixed Basis Set Embedding. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 1067-1080.	2.3	19
26	Structural and dynamic properties of liquid tin from a new modified embedded-atom method force field. <i>Physical Review B</i> , 2017, 95, .	1.1	22
27	Ab initio theory and modeling of water. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, 10846-10851.	3.3	340
28	X-ray absorption of liquid water by advanced <i>ab initio</i> methods. <i>Physical Review B</i> , 2017, 96, .	1.1	11
29	First-principles molecular dynamics study of deuterium diffusion in liquid tin. <i>Journal of Chemical Physics</i> , 2017, 147, 064505.	1.2	11
30	Characterization of the liquid Li-solid Mo (1%O) interface from classical molecular dynamics for plasma-facing applications. <i>Nuclear Fusion</i> , 2017, 57, 116036.	1.6	7
31	Prediction and characterization of an Mg-Al intermetallic compound with potentially improved ductility via orbital-free and Kohn-Sham density functional theory. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2017, 25, 075002.	0.8	11
32	Rock-salt structure lithium deuteride formation in liquid lithium with high-concentrations of deuterium: a first-principles molecular dynamics study. <i>Nuclear Fusion</i> , 2016, 56, 016020.	1.6	10
33	Suppressed gross erosion of high-temperature lithium via rapid deuterium implantation. <i>Nuclear Fusion</i> , 2016, 56, 016022.	1.6	23
34	Effect of Temperature on the Desorption of Lithium from Molybdenum(110) Surfaces: Implications for Fusion Reactor First Wall Materials. <i>Journal of Physical Chemistry B</i> , 2016, 120, 6110-6119.	1.2	15
35	Petascale Orbital-Free Density Functional Theory Enabled by Small-Box Algorithms. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 2950-2963.	2.3	41
36	Stabilization of Highly Polar $BiFeO_3$ Structure: A New Interface Design Route for Enhanced Ferroelectricity in Artificial Perovskite Superlattices. <i>Physical Review X</i> , 2016, 6, .	2.8	16

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37	Elastic and Thermodynamic Properties of Complex Mg-Al Intermetallic Compounds via Orbital-Free Density Functional Theory. <i>Physical Review Applied</i> , 2016, 5, .	1.5	30
38	Large-scale ab initio simulations based on systematically improvable atomic basis. <i>Computational Materials Science</i> , 2016, 112, 503-517.	1.4	61
39	Liquid Li structure and dynamics: A comparison between OFDFT and second nearest-neighbor embedded-atom method. <i>AIChE Journal</i> , 2015, 61, 2841-2853.	1.8	24
40	Introducing PROFESS 3.0: An advanced program for orbital-free density functional theory molecular dynamics simulations. <i>Computer Physics Communications</i> , 2015, 190, 228-230.	3.0	67
41	Introduction to first-principles simulation package ABACUS based on systematically improvable atomic orbitals. <i>Wuli Xuebao/Acta Physica Sinica</i> , 2015, 64, 187104.	0.2	2
42	The melting point of lithium: an orbital-free first-principles molecular dynamics study. <i>Molecular Physics</i> , 2013, 111, 3448-3456.	0.8	41
43	Accelerating atomic orbital-based electronic structure calculation via pole expansion and selected inversion. <i>Journal of Physics Condensed Matter</i> , 2013, 25, 295501.	0.7	50
44	Overlaying optical lattices for simulation of complex frustrated antiferromagnets. <i>Physical Review A</i> , 2012, 85, .	1.0	4
45	Substrate induced bandgap in multilayer epitaxial graphene on the 4H-SiC (0001) surface. <i>Physica Status Solidi (B): Basic Research</i> , 2011, 248, 1690-1695.	0.7	6
46	Electronic structure interpolation via atomic orbitals. <i>Journal of Physics Condensed Matter</i> , 2011, 23, 325501.	0.7	17
47	Systematically improvable optimized atomic basis sets for <i>ab initio</i> calculations. <i>Journal of Physics Condensed Matter</i> , 2010, 22, 445501.	0.7	46
48	Method to construct transferable minimal basis sets for <i>ab initio</i> calculations. <i>Physical Review B</i> , 2009, 80, .	1.1	1
49	A caveat of the charge-extrapolation scheme for modeling electrochemical reactions on semiconductor surfaces: an issue induced by a discontinuous Fermi level change. <i>Physical Chemistry Chemical Physics</i> , 0, .	1.3	1
50	Structural and Dynamic Properties of Solvated Hydroxide and Hydronium Ions in Water from Ab Initio Modeling. <i>Journal of Chemical Physics</i> , 0, .	1.2	8