Mohan Chen

List of Publications by Year
in descending order

50 papers	1,678 citations	331670 21 h-index	302126 39 g-index
50 all docs	50 docs citations	50 times ranked	1895 citing authors

#	Article	IF	Citations
1	Ab initio theory and modeling of water. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 10846-10851.	7.1	340
2	Hydroxide diffuses slower than hydronium in water because its solvated structure inhibits correlated proton transfer. Nature Chemistry, 2018, 10, 413-419.	13.6	175
3	86 PFLOPS Deep Potential Molecular Dynamics simulation of 100 million atoms with ab initio accuracy. Computer Physics Communications, 2021, 259, 107624.	7.5	100
4	Pushing the Limit of Molecular Dynamics with Ab Initio Accuracy to 100 Million Atoms with Machine Learning. , 2020, , .		69
5	Introducing PROFESS 3.0: An advanced program for orbital-free density functional theory molecular dynamics simulations. Computer Physics Communications, 2015, 190, 228-230.	7.5	67
6	Large-scale ab initio simulations based on systematically improvable atomic basis. Computational Materials Science, 2016, 112, 503-517.	3.0	61
7	Deep neural network for the dielectric response of insulators. Physical Review B, 2020, 102, .	3.2	60
8	Structural, electronic, and dynamical properties of liquid water by ab initio molecular dynamics based on SCAN functional within the canonical ensemble. Journal of Chemical Physics, 2018, 148, 164505.	3.0	58
9	Accelerating atomic orbital-based electronic structure calculation via pole expansion and selected inversion. Journal of Physics Condensed Matter, 2013, 25, 295501.	1.8	50
10	Systematically improvable optimized atomic basis sets forab initiocalculations. Journal of Physics Condensed Matter, 2010, 22, 445501.	1.8	46
11	The melting point of lithium: an orbital-free first-principles molecular dynamics study. Molecular Physics, 2013, 111, 3448-3456.	1.7	41
12	Petascale Orbital-Free Density Functional Theory Enabled by Small-Box Algorithms. Journal of Chemical Theory and Computation, 2016, 12, 2950-2963.	5.3	41
13	Modeling Liquid Water by Climbing up Jacobâ€™s Ladder in Density Functional Theory Facilitated by Using Deep Neural Network Potentials. Journal of Physical Chemistry B, 2021, 125, 11444-11456.	2.6	40
14	Electron-Hole Theory of the Effect of Quantum Nuclei on the X-Ray Absorption Spectra of Liquid Water. Physical Review Letters, 2018, 121, 137401.	7.8	35
15	Disordered hyperuniformity in two-dimensional amorphous silica. Science Advances, 2020, 6, eaba0826.	10.3	35
16	Elastic and Thermodynamic Properties of Complex Mg-Al Intermetallic Compounds via Orbital-Free Density Functional Theory. Physical Review Applied, 2016, 5, .	3.8	30
17	Stoneâ€“Wales defects preserve hyperuniformity in amorphous two-dimensional networks. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	28
18	First-principles study of the infrared spectrum in liquid water from a systematically improved description of H-bond network. Physical Review B, 2019, 99, .	3.2	27

#	Article	IF	Citations
19	Liquid li structure and dynamics: A comparison between OFDFT and second nearestâ€neighbor embeddedâ€atom method. AICHE Journal, 2015, 61, 2841-2853.	3.6	24
20	Suppressed gross erosion of high-temperature lithium via rapid deuterium implantation. Nuclear Fusion, 2016, 56, 016022.	3.5	23
21	Structural and dynamic properties of liquid tin from a new modified embedded-atom method force field. Physical Review B, 2017, 95, .	3.2	22
22	Isotope effects in molecular structures and electronic properties of liquid water via deep potential molecular dynamics based on the SCAN functional. Physical Review B, 2020, 102, .	3.2	22
23	Structure and dynamics of warm dense aluminum: a molecular dynamics study with density functional theory and deep potential. Journal of Physics Condensed Matter, 2020, 32, 144002.	1.8	21
24	Stabilization of Hydroxide Ions at the Interface of a Hydrophobic Monolayer on Water via Reduced Proton Transfer. Physical Review Letters, 2020, 125, 156803.	7.8	21
25	Potential Functional Embedding Theory at the Correlated Wave Function Level. 1. Mixed Basis Set Embedding. Journal of Chemical Theory and Computation, 2017, 13, 1067-1080.	5.3	19
26	Warm dense matter simulation via electron temperature dependent deep potential molecular dynamics. Physics of Plasmas, 2020, 27, .	1.9	19
27	Electronic structure interpolation via atomic orbitals. Journal of Physics Condensed Matter, 2011, 23, 325501.	1.8	17
28	Stabilization of Highly Polar<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>BiFeO</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn><mml:mi> Structure: A New Interface Design Route for Enhanced Ferroelectricity in Artificial Perovskite Superlattices. Physical Review X, 2016, 6, .	8.9	16
29	Orbital-free density functional theory simulation of collective dynamics coupling in liquid Sn. Journal of Chemical Physics, 2018, 149, 094504.	3.0	16
30	Effect of Temperature on the Desorption of Lithium from Molybdenum(110) Surfaces: Implications for Fusion Reactor First Wall Materials. Journal of Physical Chemistry B, 2016, 120, 6110-6119.	2.6	15
31	Finite-temperature infrared and Raman spectra of high-pressure hydrogen from first-principles molecular dynamics. Physical Review B, 2018, 98, .	3.2	14
32	Electrical and thermal transport properties of medium-entropy Si Ge Sn alloys. Acta Materialia, 2020, 199, 443-452.	7.9	13
33	Thermal transport by electrons and ions in warm dense aluminum: A combined density functional theory and deep potential study. Matter and Radiation at Extremes, 2021, 6, .	3.9	13
34	X-ray absorption of liquid water by advanced ab initio methods. Physical Review B, 2017, 96, .	3.2	11
35	First-principles molecular dynamics study of deuterium diffusion in liquid tin. Journal of Chemical Physics, 2017, 147, 064505.	3.0	11
36	Prediction and characterization of an Mg-Al intermetallic compound with potentially improved ductility via orbital-free and Kohn-Sham density functional theory. Modelling and Simulation in Materials Science and Engineering, 2017, 25, 075002.	2.0	11

#	Article	IF	Citations
37	Rock-salt structure lithium deuteride formation in liquid lithium with high-concentrations of deuterium: a first-principles molecular dynamics study. Nuclear Fusion, 2016, 56, 016020.	3.5	10
38	Structural and Dynamic Properties of Solvated Hydroxide and Hydronium Ions in Water from Ab Initio Modeling. Journal of Chemical Physics, 0, , .	3.0	8
39	Characterization of the liquid Li-solid Mo (1â€‰1â€‰0) interface from classical molecular dynamics for plasma-facing applications. Nuclear Fusion, 2017, 57, 116036.	3.5	7
40	Topological transformations in hyperuniform pentagonal two-dimensional materials induced by Stone-Wales defects. Physical Review B, 2021, 103, .	3.2	7
41	Editorial: Advances in Density Functional Theory and Beyond for Computational Chemistry. Frontiers in Chemistry, 2021, 9, 705762.	3.6	7
42	Substrate induced bandgap in multilayer epitaxial graphene on the 4Hâ€SiC ($000{ar {1}}$) surface. Physica Status Solidi (B): Basic Research, 2011, 248, 1690-1695.	1.5	6
43	Copper-doped beryllium and beryllium oxide interface: A first-principles study. Journal of Nuclear Materials, 2021, 545, 152733.	2.7	6
44	Overlaying optical lattices for simulation of complex frustrated antiferromagnets. Physical Review A, 2012, 85, .	2.5	4
45	Signature of the hydrogen-bonded environment of liquid water in X-ray emission spectra from first-principles calculations. Frontiers of Physics, 2018, 13, 1.	5.0	3
46	Orbital-free density functional theory characterization of the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msup><mml:mi>Î²</mml:mi><mml:mo>â€²</mml:mo></mml:msup><mml:mi mathvariant="normal">M</mml:mi><mml:msub><mml:mi mathvariant="normal">g</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">A</mml:mi><mml:msub><mml:mi mathvariant="normal">I</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> Samso.	2.4	3
47	Retention and recycling of deuterium in liquid lithium-tin slab studied by first-principles molecular dynamics. Journal of Nuclear Materials, 2021, 543, 152542.	2.7	2
48	Introduction to first-principles simulation package ABACUS based on systematically improvable atomic orbitals. Wuli Xuebao/Acta Physica Sinica, 2015, 64, 187104.	0.5	2
49	Method to construct transferable minimal basis sets forab initiocalculations. Physical Review B, 2009, 80, .	3.2	1
50	A caveat of the charge-extrapolation scheme for modeling electrochemical reactions on semiconductor surfaces: an issue induced by a discontinuous Fermi level change. Physical Chemistry Chemical Physics, 0, , .	2.8	1