Kohei Shimamura

List of Publications by Year
in descending order

48	647	567144 15	610775 24
papers	citations	h-index	g-index

48	48	48	714
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Thermal conductivity calculation based on Greenâ€“Kubo formula using ANN potential for Î²-Ag2Se. Journal of Physics and Chemistry of Solids, 2022, 163, 110580.	1.9	11
2	Exploring far-from-equilibrium ultrafast polarization control in ferroelectric oxides with excited-state neural network quantum molecular dynamics. Science Advances, 2022, 8, eabk2625.	4.7	8
3	Importance of Adjusting Coefficients in Cost Function for Construction of High-Accuracy Machine-Learning Interatomic Potential. Journal of the Physical Society of Japan, 2022, 91, .	0.7	0
4	Dielectric Constant of Liquid Water Determined with Neural Network Quantum Molecular Dynamics. Physical Review Letters, 2021, 126, 216403.	2.9	16
5	Neural Network Quantum Molecular Dynamics, Intermediate Range Order in GeSe₂, and Neutron Scattering Experiments. Journal of Physical Chemistry Letters, 2021, 12, 6020-6028.	2.1	2
6	Ex-NNQMD: Extreme-Scale Neural Network Quantum Molecular Dynamics. , 2021, , .		1
7	Reproduction of Melting and Crystallization of Sodium by Machine-Learning Interatomic Potential Based on Artificial Neural Networks. Journal of the Physical Society of Japan, 2021, 90, 094603.	0.7	2
8	Estimating thermal conductivity of Î±-Ag2Se using ANN potential with Chebyshev descriptor. Chemical Physics Letters, 2021, 778, 138748.	1.2	5
9	Improvement of the Force Field for Î²-d-Glucose with Machine Learning. Molecules, 2021, 26, 6691.	1.7	1
10	Molecular Dynamics Simulation of Shock Compression Behavior Based on First-Principles Calculation and Machine-Learning. Review of High Pressure Science and Technology/Koatsuryoku No Kagaku To Gijutsu, 2021, 31, 132-139.	0.1	0
11	Temperature relaxation in binary hard-sphere mixture system: Molecular dynamics and kinetic theory study. Journal of Chemical Physics, 2020, 153, 034114.	1.2	1
12	Molecular Dynamics Study of Thermal Conductivity of Silver Chalcogenides. Physica Status Solidi (B): Basic Research, 2020, 257, 2000183.	0.7	4
13	Optically Induced Three-Stage Picosecond Amorphization in Low-Temperature SrTiO₃. Journal of Physical Chemistry Letters, 2020, 11, 9605-9612.	2.1	4
14	Application of First-Principles-Based Artificial Neural Network Potentials to Multiscale-Shock Dynamics Simulations on Solid Materials. Journal of Physical Chemistry Letters, 2020, 11, 4536-4541.	2.1	12
15	Computational and training requirements for interatomic potential based on artificial neural network for estimating low thermal conductivity of silver chalcogenides. Journal of Chemical Physics, 2020, 153, 234301.	1.2	13
16	QXMD: An open-source program for nonadiabatic quantum molecular dynamics. SoftwareX, 2019, 10, 100307.	1.2	32
17	Hydrogen Bond Preserving Stress Release Mechanism Is Key to the Resilience of Aramid Fibers. Journal of Physical Chemistry B, 2019, 123, 9719-9723.	1.2	6
18	Guidelines for creating artificial neural network empirical interatomic potential from first-principles molecular dynamics data under specific conditions and its application to Î±-Ag2Se. Journal of Chemical Physics, 2019, 151, 124303.	1.2	19

#	Article	IF	Citations
19	Thermodynamic integration by neural network potentials based on first-principles dynamic calculations. Physical Review B, 2019, 100, .	1.1	10
20	Ab initio molecular dynamics study of prebiotic production processes of organic compounds at meteorite impacts on ocean. Journal of Computational Chemistry, 2019, 40, 349-359.	1.5	5
21	Meteorite impacts on ancient oceans opened up multiple NH₃ production pathways. Physical Chemistry Chemical Physics, 2017, 19, 11655-11667.	1.3	5
22	Rotation mechanism of methylammonium molecules in organometal halide perovskite in cubic phase: An ab initio molecular dynamics study. Journal of Chemical Physics, 2016, 145, 224503.	1.2	14
23	Meteorite Impact-Induced Rapid NH3 Production on Early Earth: Ab Initio Molecular Dynamics Simulation. Scientific Reports, 2016, 6, 38953.	1.6	14
24	The nature of free-carrier transport in organometal halide perovskites. Scientific Reports, 2016, 6, 19599.	1.6	38
25	Anisotropic mechanoresponse of energetic crystallites: a quantum molecular dynamics study of nano-collision. Nanoscale, 2016, 8, 9714-9720.	2.8	2
26	Nanocarbon synthesis by high-temperature oxidation of nanoparticles. Scientific Reports, 2016, 6, 24109.	1.6	15
27	Crystalline anisotropy of shock-induced phenomena: Omni-directional multiscale shock technique. Applied Physics Letters, 2016, 108, .	1.5	13
28	Role of oxygen vacancy in dissociation of oxygen molecule on SOFC cathode: Ab initio molecular dynamics simulation. Solid State Ionics, 2016, 285, 209-214.	1.3	19
29	Reactive Molecular Dynamics Simulations, Data Analytics and Visualization. Materials Research Society Symposia Proceedings, 2015, 1756, 1.	0.1	0
30	A crossover in anisotropic nanomechanochemistry of van der Waals crystals. Applied Physics Letters, 2015, 107, .	1.5	11
31	Reaction of ethylene molecules with a nickel cluster: <i>ab initio</i> molecular dynamics study. Transactions of the Materials Research Society of Japan, 2015, 40, 215-218.	0.2	1
32	Enhanced charge recombination due to surfaces and twin defects in GaAs nanostructures. Journal of Applied Physics, 2015, 117, 054307.	1.1	16
33	Ab Initio Molecular Dynamics Simulation of Ethylene Reaction on Nickel (111) Surface. Journal of Physical Chemistry C, 2015, 119, 3210-3216.	1.5	22
34	Ab initio molecular dynamics simulation of ethanol decomposition on platinum cluster at initial stage of carbon nanotube growth. Chemical Physics Letters, 2015, 636, 110-116.	1.2	10
35	First principles calculation of CH4 decomposition on nickel (111) surface. European Physical Journal B, 2015, 88, 1.	0.6	14
36	Oxygen 2p Partial Density of States in a Typical Oxide Glass B₂O₃. Journal of the Physical Society of Japan, 2014, 83, 114601.	0.7	4

#	Article	IF	Citations
37	Metascalable Quantum Molecular Dynamics Simulations of Hydrogen-on-Demand. , 2014, , .		8
38	A divide-conquer-recombine algorithmic paradigm for large spatiotemporal quantum molecular dynamics simulations. Journal of Chemical Physics, 2014, 140, 18A529.	1.2	57
39	Rapid hydrogen production from water using aluminum nanoclusters: A quantum molecular dynamics simulation study. Solid State Ionics, 2014, 262, 908-910.	1.3	4
40	Hydrogen-on-Demand Using Metallic Alloy Nanoparticles in Water. Nano Letters, 2014, 14, 4090-4096.	4.5	33
41	Low reactivity of methane on copper surface during graphene synthesis via CVD process: Ab initio molecular dynamics simulation. Chemical Physics Letters, 2014, 610-611, 33-38.	1.2	19
42	Bond dissociation mechanism of ethanol during carbon nanotube synthesis via alcohol catalytic CVD technique: Ab initio molecular dynamics simulation. Chemical Physics Letters, 2014, 595-596, 185-191.	1.2	27
43	Divide-Conquer-Recombine. , 2014, , .		3
44	Bonding and Structure of Ceramic-Ceramic Interfaces. Physical Review Letters, 2013, 111, 066103.	2.9	16
45	Critical size for the generation of misfit dislocations and their effects on electronic properties in GaAs nanosheets on Si substrate. Journal of Applied Physics, 2013, 114, 074316.	1.1	3
46	Effects of twins on the electronic properties of GaAs. Applied Physics Letters, 2013, 103, 022105.	1.5	42
47	Ab initio molecular dynamics simulation of dissociation of methane on nickel(1 1 1) surface: Unravelling initial stage of graphene growth via a CVD technique. Chemical Physics Letters, 2013, 565, 92-97.	1.2	54
48	Ab Initio Molecular Dynamics Simulation of the Dissociation of Ethanol on a Nickel Cluster: Understanding the Initial Stage of Metal-Catalyzed Growth of Carbon Nanotubes. Journal of Physical Chemistry C, 2013, 117, 9983-9990.	1.5	31