Akihide Koura

List of Publications by Year
in descending order

18 papers	124 citations	1307594 7 h-index	1281871 11 g-index
18 all docs	18 docs citations	18 times ranked	122 citing authors

#	Article	IF	Citations
1	Guidelines for creating artificial neural network empirical interatomic potential from first-principles molecular dynamics data under specific conditions and its application to α-Ag2Se. Journal of Chemical Physics, 2019, 151, 124303.	3.0	19
2	*Ab initio* simulation of permanent densification in silica glass. Physical Review B, 2017, 96, .	3.2	16
3	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.	3.0	13
4	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.	4.6	12
5	Thermal conductivity calculation based on Green–Kubo formula using ANN potential for β-Ag2Se. Journal of Physics and Chemistry of Solids, 2022, 163, 110580.	4.0	11
6	Local Clusters in a Distorted Rocksalt GeTe Crystal Found by X-ray Fluorescence Holography. Journal of the Physical Society of Japan, 2014, 83, 124602.	1.6	10
7	Thermodynamic integration by neural network potentials based on first-principles dynamic calculations. Physical Review B, 2019, 100, .	3.2	10
8	GGA+U Molecular Dynamics Study of Structural and Dynamic Properties of Superionic Conductor Ag_2Se. Journal of the Physical Society of Japan, 2019, 88, 115002.	1.6	7
9	Structural Changes of Short- and Intermediate-Range Order in Liquid Arsenic under Pressure. Journal of the Physical Society of Japan, 2015, 84, 094602.	1.6	5
10	Estimating thermal conductivity of α-Ag2Se using ANN potential with Chebyshev descriptor. Chemical Physics Letters, 2021, 778, 138748.	2.6	5
11	Intermediate range structure of amorphous Cu_2GeTe_3: *ab initio* molecular dynamics study. Journal of Physics Condensed Matter, 2020, 32, 244001.	1.8	5
12	Dynamic asymmetry of self-diffusion in liquid ZnCl2 under pressure: An ab initio molecular-dynamics study. Journal of Chemical Physics, 2013, 138, 134504.	3.0	4
13	Molecular Dynamics Study of Thermal Conductivity of Silver Chalcogenides. Physica Status Solidi (B): Basic Research, 2020, 257, 2000183.	1.5	4
14	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.	1.6	2
15	Static Structure of Liquid GeSe Under Pressure: Ab Initio Molecular Dynamics Simulations. Physica Status Solidi (B): Basic Research, 2018, 255, 1800103.	1.5	1
16	Concentration Dependence of the Dynamic Properties of Liquid Tl_xSe_{1-x} Based on Ab initio Molecular-Dynamics Simulations. Journal of the Physical Society of Japan, 2013, 82, 094602.	1.6	0
17	First-Principles Study of the Adsorption/Dissociation Reactions of Water on a Fe- and $Co-Al_2O_4$ Cluster. E-Journal of Surface Science and Nanotechnology, 2015, 13, 410-412.	0.4	0
18	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, .	1.6	0