Hideo Doi

List of Publications by Year
in descending order

22	226	1040056 9	1058476 14
papers	citations	h-index	g-index

22	22	22	155
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Screening toward the Development of Fingerprints of Atomic Environments Using Bond-Orientational Order Parameters. ACS Omega, 2022, 7, 4606-4613.	3.5	2
2	Searching local order parameters to classify water structures of ice Ih, Ic, and liquid. Journal of Chemical Physics, 2021, 154, 164505.	3.0	13
3	Searching for local order parameters to classify water structures at triple points. Journal of Computational Chemistry, 2021, 42, 1720-1727.	3.3	6
4	Mining of Effective Local Order Parameters to Classify Ice Polymorphs. Journal of Physical Chemistry A, 2021, 125, 9518-9526.	2.5	6
5	Stabilization Mechanism for a Nonfibrillar Amyloid Î² Oligomer Based on Formation of a Hydrophobic Core Determined by Dissipative Particle Dynamics. ACS Chemical Neuroscience, 2020, 11, 385-394.	3.5	15
6	Folding simulation of small proteins by dissipative particle dynamics (DPD) with non-empirical interaction parameters based on fragment molecular orbital calculations. Applied Physics Express, 2020, 13, 017002.	2.4	17
7	Mining of effective local order parameters for classifying crystal structures: A machine learning study. Journal of Chemical Physics, 2020, 152, 214501.	3.0	14
8	Ab Initio Fragment Molecular Orbital-Based Molecular Dynamics (FMO-MD) Simulations of (NH3)32 Cluster: Effects of Electron Correlation. Bulletin of the Chemical Society of Japan, 2020, 93, 553-560.	3.2	1
9	Machine learning-aided analysis for complex local structure of liquid crystal polymers. Scientific Reports, 2019, 9, 16370.	3.3	27
10	Fragment Molecular Orbital Based Parametrization Procedure for Mesoscopic Structure Prediction of Polymeric Materials. Journal of Physical Chemistry B, 2018, 122, 338-347.	2.6	20
11	Theoretical analyses on water cluster structures in polymer electrolyte membrane by using dissipative particle dynamics simulations with fragment molecular orbital based effective parameters. RSC Advances, 2018, 8, 34582-34595.	3.6	26
12	Formation Mechanism of Lipid Membrane and Vesicle Using Small Angle X-ray Scattering and Dissipative Particle Dynamics (DPD) Method. Journal of Computer Chemistry Japan, 2018, 17, 172-179.	0.1	6
13	An automated framework to evaluate effective interactionparameters for dissipative particle dynamics simulations basedon the fragment molecular orbital (FMO) method. Journal of Computer Chemistry Japan, 2018, 17, 102-109.	0.1	9
14	Application of TensorFlow to recognition of visualized results of fragment molecular orbital (FMO) calculations. Chem-Bio Informatics Journal, 2018, 18, 58-69.	0.3	6
15	Replica exchange molecular simulation of Lennardâ€“Jones particles in a two-dimensional confined system. AIP Advances, 2017, 7, .	1.3	4
16	Dissipative particle dynamics (DPD) simulations with fragment molecular orbital (FMO) based effective parameters for 1-Palmitoyl-2-oleoyl phosphatidyl choline (POPC) membrane. Chemical Physics Letters, 2017, 684, 427-432.	2.6	29
17	Development and Performance Evaluation of a Simulation Code for Dissipative Particle Dynamics (DPD) CAMUS. Journal of Computer Chemistry Japan, 2017, 16, 126-128.	0.1	2
18	A New Treatment for Water near the Interface between Lipid Membrane and Silica in Dissipative Particle Dynamics Simulation. Journal of Computer Chemistry Japan, 2017, 16, 28-31.	0.1	8

#	Article	IF	Citations
19	Approaches for Controlling the Temperature and Pressure Range in Generalized NPT Ensembles. Journal of Chemical Theory and Computation, 2015, 11, 4370-4376.	5.3	0
20	A new variant of multicanonical Monte Carlo algorithm with specifying the temperature range and its application to the hydration free energy change of fluorinated methane derivatives. Chemical Physics Letters, 2014, 595-596, 55-60.	2.6	3
21	Influence of Trimethylamine N-Oxide (TMAO) on the Three-dimensional Distribution and Alignment of Solvent Molecules in Aqueous Solution. Chemistry Letters, 2014, 43, 865-867.	1.3	10
22	Hydration of Adamantane Skeleton: Water Assembling around Amantadine and Halo-substituted Adamantanes. Chemistry Letters, 2013, 42, 292-294.	1.3	2