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	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
2	Machine learning-aided analysis for complex local structure of liquid crystal polymers. Scientific Reports, 2019, 9, 16370.	3.3	27
3	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
4	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
5	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
6	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
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	Searching local order parameters to classify water structures of ice Ih, Ic, and liquid. Journal of Chemical Physics, 2021, 154, 164505.	3.0	13
9	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
10	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
11	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
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	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
14	Searching for local order parameters to classify water structures at triple points. Journal of Computational Chemistry, 2021, 42, 1720-1727.	3.3	6
15	Mining of Effective Local Order Parameters to Classify Ice Polymorphs. Journal of Physical Chemistry A, 2021, 125, 9518-9526.	2.5	6
16	Replica exchange molecular simulation of Lennardâ€“Jones particles in a two-dimensional confined system. AIP Advances, 2017, 7, .	1.3	4
17	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
18	Hydration of Adamantane Skeleton: Water Assembling around Amantadine and Halo-substituted Adamantanes. Chemistry Letters, 2013, 42, 292-294.	1.3	2

#	Article	IF	Citations
19	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
20	Screening toward the Development of Fingerprints of Atomic Environments Using Bond-Orientational Order Parameters. ACS Omega, 2022, 7, 4606-4613.	3.5	2
21	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
22	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