

Kazuaki Z Takahashi

List of Publications by Year in descending order

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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	Trade-off effect between the stress and strain range in the soft elasticity of liquid crystalline elastomers. Polymer Journal, 2022, 54, 1017-1027.	2.7	3
3	Searching local order parameters to classify water structures of ice Ih, Ic, and liquid. Journal of Chemical Physics, 2021, 154, 164505.	3.0	13
4	Searching for local order parameters to classify water structures at triple points. Journal of Computational Chemistry, 2021, 42, 1720-1727.	3.3	6
5	Molecular architecture dependence of mesogen rotation during uniaxial elongation of liquid crystal elastomers. Polymer, 2021, 229, 123970.	3.8	7
6	Multistep nucleation of anisotropic molecules. Nature Communications, 2021, 12, 5278.	12.8	23
7	Mining of Effective Local Order Parameters to Classify Ice Polymorphs. Journal of Physical Chemistry A, 2021, 125, 9518-9526.	2.5	6
8	Mining of effective local order parameters for classifying crystal structures: A machine learning study. Journal of Chemical Physics, 2020, 152, 214501.	3.0	14
9	Performance of Coarse Graining in Estimating Polymer Properties: Comparison with the Atomistic Model. Polymers, 2020, 12, 382.	4.5	7
10	Machine learning-aided analysis for complex local structure of liquid crystal polymers. Scientific Reports, 2019, 9, 16370.	3.3	27
11	Critical test of isotropic periodic sum techniques with group-based cut-off schemes. Scientific Reports, 2018, 8, 4185.	3.3	6
12	Development of Coarse-Grained Liquid-Crystal Polymer Model with Efficient Electrostatic Interaction: Toward Molecular Dynamics Simulations of Electroactive Materials. Materials, 2018, 11, 83.	2.9	10
13	A fast and accurate computational method for the linear-combination-based isotropic periodic sum. Scientific Reports, 2018, 8, 11880.	3.3	2
14	Combined use of periodic reaction field and coarse-grained molecular dynamics simulations. I. phospholipid monolayer systems. Molecular Simulation, 2017, 43, 971-976.	2.0	1
15	Critical test of bead-spring model to resolve the scaling laws of polymer melts: a molecular dynamics study. Molecular Simulation, 2017, 43, 1196-1201.	2.0	8
16	Onset of static and dynamic universality among molecular models of polymers. Scientific Reports, 2017, 7, 12379.	3.3	15
17	Molecular Dynamics Simulations for Resolving Scaling Laws of Polyethylene Melts. Polymers, 2017, 9, 24.	4.5	25
18	Comparison of the accuracy of periodic reaction field methods in molecular dynamics simulations of a model liquid crystal system. Journal of Computational Chemistry, 2015, 36, 2406-2411.	3.3	6

#	ARTICLE	IF	CITATIONS
19	An improvement of truncation method by a novel reaction field: Accurate computation for estimating methanol liquid-vapor interfacial systems. <i>Computational Materials Science</i> , 2015, 100, 191-194.	3.0	3
20	Application of isotropic periodic sum method for 4-pentyl-4'-cyanobiphenyl liquid crystal. <i>Molecular Simulation</i> , 2015, 41, 927-935.	2.0	8
21	A determination of liquid-vapour interfacial properties for methanol using a linear-combination-based isotropic periodic sum. <i>Molecular Simulation</i> , 2015, 41, 795-800.	2.0	4
22	Design of a reaction field using a linear-combination-based isotropic periodic sum method. <i>Journal of Computational Chemistry</i> , 2014, 35, 865-875.	3.3	10
23	Truncation Effects of Shift Function Methods in Bulk Water Systems. <i>Entropy</i> , 2013, 15, 3249-3264.	2.2	14
24	Molecular dynamics study on structural change in the surface membrane of an insonified coated microbubble. , 2012, , .		0
25	An Improved Isotropic Periodic Sum Method That Uses Linear Combinations of Basis Potentials. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 4503-4516.	5.3	16
26	Cut-off radius effect of the isotropic periodic sum method for polar molecules in a bulk water system. <i>Molecular Simulation</i> , 2012, 38, 397-403.	2.0	12
27	Cutoff radius effect of the isotropic periodic sum and Wolf method in liquid-vapor interfaces of water. <i>Journal of Chemical Physics</i> , 2011, 134, 174112.	3.0	39
28	A combination of the tree-code and IPS method to simulate large scale systems by molecular dynamics. <i>Journal of Chemical Physics</i> , 2011, 135, 174108.	3.0	19
29	Cutoff Radius Effect of Water Configuration Using the Wolf Method. , 2011, , .		0
30	Cutoff radius effect of the isotropic periodic sum method in homogeneous system. II. Water. <i>Journal of Chemical Physics</i> , 2010, 133, 014109.	3.0	32
31	Cutoff radius effect of isotropic periodic sum method for transport coefficients of Lennard-Jones liquid. <i>Journal of Chemical Physics</i> , 2007, 127, 114511.	3.0	28