Kenji Yasuoka

List of Publications by Year
in descending order

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193	5,047	76294	114418
papers	citations	40 h-index	63 g-index

197	197	197	5035
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Coexistence and transition between Cassie and Wenzel state on pillared hydrophobic surface. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 8435-8440.	3.3	395
2	Molecular dynamics of homogeneous nucleation in the vapor phase. I. Lennard-Jones fluid. Journal of Chemical Physics, 1998, 109, 8451-8462.	1.2	259
3	Water proton configurations in structures I, II, and H clathrate hydrate unit cells. Journal of Chemical Physics, 2013, 138, 124504.	1.2	193
4	Measurement of Contact-Angle Hysteresis for Droplets on Nanopillared Surface and in the Cassie and Wenzel States: A Molecular Dynamics Simulation Study. ACS Nano, 2011, 5, 6834-6842.	7.3	152
5	Statistical Study of Clathrate-Hydrate Nucleation in a Water/Hydrochlorofluorocarbon System:Â Search for the Nature of the â€œMemory Effectâ€• Journal of Physical Chemistry B, 2003, 107, 5289-5293.	1.2	149
6	Molecular dynamics of homogeneous nucleation in the vapor phase. II. Water. Journal of Chemical Physics, 1998, 109, 8463-8470.	1.2	130
7	Evaporation and condensation at a liquid surface. I. Argon. Journal of Chemical Physics, 1994, 101, 7904-7911.	1.2	89
8	Self-Assembly of Surfactants and Polymorphic Transition in Nanotubes. Journal of the American Chemical Society, 2008, 130, 7916-7920.	6.6	87
9	Non-Gaussian Fluctuations Resulting from Power-Law Trapping in a Lipid Bilayer. Physical Review Letters, 2011, 107, 178103.	2.9	87
10	Molecular Mechanisms of How Mercury Inhibits Water Permeation through Aquaporin-1: Understanding by Molecular Dynamics Simulation. Biophysical Journal, 2010, 98, 1512-1519.	0.2	86
11	Origin of subdiffusion of water molecules on cell membrane surfaces. Scientific Reports, 2014, 4, 4720.	1.6	84
12	Structure of cold nuclear matter at subnuclear densities by quantum molecular dynamics. Physical Review C, 2003, 68, .	1.1	80
13	Phase diagram of nuclear â€œpastaâ€•and its uncertainties in supernova cores. Physical Review C, 2008, 77, .	1.1	77
14	From kesterite to stannite photovoltaics: Stability and band gaps of the Cu2(Zn,Fe)SnS4 alloy. Applied Physics Letters, 2014, 104, .	1.5	76
15	Formation of Nuclear â€œPastaâ€•in Supernovae. Physical Review Letters, 2009, 103, 121101.	2.9	69
16	Interactions of Pleckstrin Homology Domains with Membranes: Adding Back the Bilayer via High-Throughput Molecular Dynamics. Structure, 2016, 24, 1421-1431.	1.6	68
17	Evaporation and condensation at a liquid surface. II. Methanol. Journal of Chemical Physics, 1994, 101, 7912-7917.	1.2	67
18	Oxygen vacancy-originated highly active electrocatalysts for the oxygen evolution reaction. Journal of Materials Chemistry A, 2018, 6, 15102-15109.	5.2	67

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19	A systematic study of polarons due to oxygen vacancy formation at the rutile TiO₂(110) surface by GGA +Uand HSE06 methods. Journal of Physics Condensed Matter, 2012, 24, 435504.	0.7	63
20	A smooth-particle mesh Ewald method for DL_POLY molecular dynamics simulation package on the Fujitsu VPP700. Journal of Computational Chemistry, 2000, 21, 1187-1191.	1.5	62
21	Hardware accelerator for molecular dynamics: MDGRAPE-2. Computer Physics Communications, 2003, 155, 115-131.	3.0	60
22	Molecular dynamics simulations of vapor/liquid coexistence using the nonpolarizable water models. Journal of Chemical Physics, 2011, 134, 124708.	1.2	60
23	Diffusive Nature of Xenon Anesthetic Changes Properties of a Lipid Bilayer: Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2012, 116, 8989-8995.	1.2	59
24	Dynamic interactions between a membrane binding protein and lipids induce fluctuating diffusivity. Science Advances, 2017, 3, e1601871.	4.7	59
25	Nucleation rate analysis of methane hydrate from molecular dynamics simulations. Faraday Discussions, 2015, 179, 463-474.	1.6	57
26	Thermodynamic properties of methane/water interface predicted by molecular dynamics simulations. Journal of Chemical Physics, 2011, 134, 144702.	1.2	55
27	Microscopic study of slablike and rodlike nuclei:â€ƒQuantum molecular dynamics approach. Physical Review C, 2002, 66, .	1.1	52
28	Phases of hot nuclear matter at subnuclear densities. Physical Review C, 2004, 69, .	1.1	52
29	Free-energy calculation of structure-H hydrates. Journal of Chemical Physics, 2006, 124, 024510.	1.2	52
30	Petascale turbulence simulation using a highly parallel fast multipole method on GPUs. Computer Physics Communications, 2013, 184, 445-455.	3.0	51
31	A vesicle cell under collision with a Janus or homogeneous nanoparticle: translocation dynamics and late-stage morphology. Nanoscale, 2013, 5, 9089.	2.8	50
32	Extended study of molecular dynamics simulation of homogeneous vapor-liquid nucleation of water. Journal of Chemical Physics, 2007, 127, 214507.	1.2	49
33	Spontaneous self-assembly process for threadlike micelles. Journal of Chemical Physics, 2007, 126, 244905.	1.2	47
34	Large-scale molecular-dynamics simulation of nanoscale hydrophobic interaction and nanobubble formation. Journal of Chemical Physics, 2005, 123, 204707.	1.2	46
35	Structures of water molecules in carbon nanotubes under electric fields. Journal of Chemical Physics, 2015, 142, 124701.	1.2	45
36	Impact of nuclear â€œpastaâ€•on neutrino transport in collapsing stellar cores. Physical Review C, 2007, 75, .	1.1	44

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37	Molecular vibrations of methane molecules in the structure I clathrate hydrate from ab initio molecular dynamics simulation. Journal of Chemical Physics, 2012, 136, 044508.	1.2	43
38	Self-Assembly of Janus Oligomers into Onion-like Vesicles with Layer-by-Layer Water Discharging Capability: A Minimalist Model. ACS Nano, 2016, 10, 8026-8037.	7.3	43
39	Evidence of low-density and high-density liquid phases and isochore end point for water confined to carbon nanotube. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 4066-4071.	3.3	42
40	Water Confined in the Local Field of Ions. ChemPhysChem, 2014, 15, 4077-4086.	1.0	40
41	Molecular Dynamics Simulation of Water Nanodroplet Bounce Back from Flat and Nanopillared Surface. Langmuir, 2017, 33, 10184-10192.	1.6	40
42	Cutoff radius effect of the isotropic periodic sum and Wolf method in liquidâ€“vapor interfaces of water. Journal of Chemical Physics, 2011, 134, 174112.	1.2	39
43	Anomalous Dynamics of a Lipid Recognition Protein on a Membrane Surface. Scientific Reports, 2016, 5, 18245.	1.6	38
44	Cage occupancy of methane hydrates from Gibbs ensemble Monte Carlo simulations. Fluid Phase Equilibria, 2016, 413, 242-248.	1.4	36
45	Stability of Excess Electrons Introduced by Ti Interstitial in Rutile TiO₂(110) Surface. Journal of Physical Chemistry C, 2017, 121, 1602-1607.	1.5	36
46	Waterâ€“methanol separation with carbon nanotubes and electric fields. Nanoscale, 2015, 7, 12659-12665.	2.8	33
47	Separation of waterâ€“ethanol solutions with carbon nanotubes and electric fields. Physical Chemistry Chemical Physics, 2016, 18, 33310-33319.	1.3	33
48	Large scale molecular dynamics simulation of nucleation in supercooled NaCl. Journal of Chemical Physics, 2003, 119, 11298-11305.	1.2	32
49	Molecular dynamics of homogeneous nucleation in the vapor phase of Lennard-Jones. III. Effect of carrier gas pressure. Journal of Chemical Physics, 2007, 126, 124320.	1.2	32
50	Vibrational modes of methane in the structure H clathrate hydrate from ab initio molecular dynamics simulation. Journal of Chemical Physics, 2012, 137, 144306.	1.2	32
51	Bipolaron Formation Induced by Oxygen Vacancy at Rutile TiO₂(110) Surfaces. Journal of Physical Chemistry C, 2014, 118, 9429-9435.	1.5	31
52	Tyr-317 Phosphorylation Increases Shc Structural Rigidity and Reduces Coupling of Domain Motions Remote from the Phosphorylation Site as Revealed by Molecular Dynamics Simulations. Journal of Biological Chemistry, 2004, 279, 4657-4662.	1.6	30
53	Phase diagram of Lennard-Jones fluid confined in slit pores. Chemical Physics Letters, 2010, 490, 165-171.	1.2	29
54	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.	1.2	29

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55	Water Molecules in a Carbon Nanotube under an Applied Electric Field at Various Temperatures and Pressures. Water (Switzerland), 2017, 9, 473.	1.2	29
56	Cutoff radius effect of isotropic periodic sum method for transport coefficients of Lennard-Jones liquid. Journal of Chemical Physics, 2007, 127, 114511.	1.2	28
57	Nanoparticle Growth Analysis by Molecular Dynamics: Spherical Seed. Journal of Physical Chemistry B, 2011, 115, 10631-10645.	1.2	28
58	Self-assembly behaviours of primitive and modern lipid membrane solutions: a coarse-grained molecular simulation study. Physical Chemistry Chemical Physics, 2016, 18, 19426-19432.	1.3	28
59	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>1</mml:mn><mml:mo>/</mml:mo><mml:mi>f</mml:mi> of amino acids regulate water transportation in aquaporin 1. Physical Review E, 2014, 89, 022718.	0.8	27
60	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.	1.7	26
61	New Computational Approach to Determine Liquidâ€“Solid Phase Equilibria of Water Confined to Slit Nanopores. Journal of Chemical Theory and Computation, 2013, 9, 3299-3310.	2.3	25
62	Liquid-solid and solid-solid phase transition of monolayer water: High-density rhombic monolayer ice. Journal of Chemical Physics, 2014, 140, 184507.	1.2	25
63	Molecular Dynamics Simulations for Resolving Scaling Laws of Polyethylene Melts. Polymers, 2017, 9, 24.	2.0	25
64	Molecular Dynamics Simulation of Dissociation Process for Methane Hydrate. Annals of the New York Academy of Sciences, 2000, 912, 678-684.	1.8	24
65	A molecular dynamics study of guestâ€“host hydrogen bonding in alcohol clathrate hydrates. Physical Chemistry Chemical Physics, 2015, 17, 12639-12647.	1.3	24
66	Nanochannel with Uniform and Janus Surfaces: Shear Thinning and Thickening in Surfactant Solution. Langmuir, 2012, 28, 2866-2872.	1.6	23
67	Power-law trapping of water molecules on the lipid-membrane surface induces water retardation. Physical Review E, 2013, 87, 052715.	0.8	23
68	Origin of the blueshift of water molecules at interfaces of hydrophilic cyclic compounds. Science Advances, 2017, 3, e1701400.	4.7	22
69	Molecular dynamics simulations of ureaâ€“water binary droplets on flat and pillared hydrophobic surfaces. Faraday Discussions, 2010, 146, 185.	1.6	20
70	Nanoparticle Growth Analysis by Molecular Dynamics: Cubic Seed. Journal of Physical Chemistry B, 2012, 116, 14637-14649.	1.2	20
71	Dynamic interactions of cations, water and lipids and influence on membrane fluidity. Journal of Membrane Science, 2013, 435, 130-136.	4.1	20
72	Kinetic analysis of homogeneous droplet nucleation using large-scale molecular dynamics simulations. Journal of Chemical Physics, 2018, 149, 044504.	1.2	20

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73	Molecular dynamics simulation of homogeneous nucleation in supersaturated water vapor. Fluid Phase Equilibria, 1998, 144, 369-376.	1.4	19
74	Thermodynamic Simulations of Isobaric Hydrate-Forming Operations:â€‰ Formulation of Computational Scheme and Its Application to Hydrate Formation from a Methane + Ethane + Propane Mixture. Energy & Fuels, 2005, 19, 1587-1597.	2.5	19
75	Size-Dependent Phase Changes in Water Clusters. Journal of Chemical Theory and Computation, 2011, 7, 3083-3087.	2.3	19
76	A combination of the tree-code and IPS method to simulate large scale systems by molecular dynamics. Journal of Chemical Physics, 2011, 135, 174108.	1.2	19
77	Cage occupancies, lattice constants, and guest chemical potentials for structure II hydrogen clathrate hydrate from Gibbs ensemble Monte Carlo simulations. Journal of Chemical Physics, 2019, 150, 134503.	1.2	19
78	Natural quantum reservoir computing for temporal information processing. Scientific Reports, 2022, 12, 1353.	1.6	19
79	Molecular Dynamics Study on Class A Î²-Lactamase: Hydrogen Bond Network among the Functional Groups of Penicillin G and Side Chains of the Conserved Residues in the Active Site. Journal of Physical Chemistry B, 2003, 107, 10274-10283.	1.2	18
80	Hydrogen-Bonded Clusters on the Vapor/Ethanol-Aqueous-Solution Interface. Journal of Physical Chemistry B, 2006, 110, 23264-23273.	1.2	18
81	Understanding Molecular Motor Walking along a Microtubule: A Themosensitive Asymmetric Brownian Motor Driven by Bubble Formation. Journal of the American Chemical Society, 2013, 135, 8616-8624.	6.6	18
82	Molecular Insight into Different Denaturing Efficiency of Urea, Guanidinium, and Methanol: A Comparative Simulation Study. Journal of Chemical Theory and Computation, 2013, 9, 2540-2551.	2.3	18
83	Energy science of clathrate hydrates: Simulation-based advances. MRS Bulletin, 2011, 36, 205-210.	1.7	17
84	Thermodynamic stability of type-I and type-II clathrate hydrates depending on the chemical species of the guest substances. Journal of Chemical Physics, 2007, 126, 234506.	1.2	16
85	Current performance gains from utilizing the GPU or the ASIC MDGRAPEâ€3 within an enhanced Poisson Boltzmann approach. Journal of Computational Chemistry, 2009, 30, 2351-2357.	1.5	16
86	An Improved Isotropic Periodic Sum Method That Uses Linear Combinations of Basis Potentials. Journal of Chemical Theory and Computation, 2012, 8, 4503-4516.	2.3	16
87	Subsurface Polaron Concentration As a Factor in the Chemistry of Reduced TiO₂ (110) Surfaces. Journal of Physical Chemistry C, 2017, 121, 11325-11334.	1.5	16
88	Analysis of three-phase equilibrium conditions for methane hydrate by isometric-isothermal molecular dynamics simulations. Journal of Chemical Physics, 2018, 148, 184501.	1.2	16
89	Statistical-Thermodynamics Modeling of Clathrate-Hydrate-Forming Systems Suitable as Working Media of a Hydrate-Based Refrigeration System. International Journal of Thermophysics, 2009, 30, 1838-1852.	1.0	15
90	Poisson property of the occurrence of flip-flops in a model membrane. Journal of Chemical Physics, 2014, 140, 064901.	1.2	15

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91	Onset of static and dynamic universality among molecular models of polymers. Scientific Reports, 2017, 7, 12379.	1.6	15
92	Asymmetric Brownian Motor Driven by Bubble Formation in a Hydrophobic Channel. ACS Nano, 2010, 4, 5905-5913.	7.3	14
93	Observation of Interstitial Molecular Hydrogen in Clathrate Hydrates. Angewandte Chemie - International Edition, 2014, 53, 10710-10713.	7.2	14
94	Origin of 1/f noise in hydration dynamics on lipid membrane surfaces. Scientific Reports, 2015, 5, 8876.	1.6	14
95	Water permeation through the internal water pathway in activated GPCR rhodopsin. PLoS ONE, 2017, 12, e0176876.	1.1	14
96	Predicting Thermodynamic Stability of Clathrate Hydrates Based on Molecular-Dynamics Simulations and Its Confirmation by Phase-Equilibrium Measurements. Journal of Physical Chemistry C, 2007, 111, 3799-3802.	1.5	13
97	Microscopic insights into nucleation in a sulfuric acidâ€“water vapor mixture based on molecular dynamics simulation. Journal of Chemical Physics, 2009, 130, 104705.	1.2	13
98	Phase behaviors of deeply supercooled bilayer water unseen in bulk water. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 4839-4844.	3.3	13
99	Differences in ligand-induced protein dynamics extracted from an unsupervised deep learning approach correlate with proteinâ€“ligand binding affinities. Communications Biology, 2022, 5, 481.	2.0	13
100	Molecular Dynamics Simulations of Prion Proteins-Effect of Ala117 .RAR.Val mutation-. Chem-Bio Informatics Journal, 2003, 3, 1-11.	0.1	12
101	Cut-off radius effect of the isotropic periodic sum method for polar molecules in a bulk water system. Molecular Simulation, 2012, 38, 397-403.	0.9	12
102	Suppression of lattice thermal conductivity by mass-conserving cation mutation in multi-component semiconductors. APL Materials, 2016, 4, 104809.	2.2	12
103	Crystal Engineering of Bi₂WO₆ to Polar Aurivillius-Phase Oxyhalides. Journal of Physical Chemistry C, 2019, 123, 29155-29161.	1.5	12
104	Anisotropic molecular clustering in liquid ethanol induced by a charged fully hydroxylated silicon dioxide (SiO2) surface. Chemical Physics Letters, 2007, 448, 253-257.	1.2	11
105	Liquidâ€“solid phase transitions of Lennard-Jones particles confined to slit pores: towards the construction of temperatureâ€“pressure-slit width phase diagram. Molecular Simulation, 2012, 38, 373-377.	0.9	11
106	Phase diagrams of confined solutions of dimyristoylphosphatidylcholine (DMPC) lipid and cholesterol in nanotubes. Microfluidics and Nanofluidics, 2013, 14, 995-1010.	1.0	11
107	Evaporation and Condensation as a Unimolecular Chemical Reaction: Does the Potential Barrier Exist at a Molecular Liquid Surface ?. Bulletin of the Chemical Society of Japan, 1994, 67, 859-862.	2.0	10
108	Fast Calculation of Electrostatic Potentials on the GPU or the ASIC MD-GRAPE-3. Computer Journal, 2011, 54, 1181-1187.	1.5	10

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109	The acidic tail of HMGB1 regulates its secondary structure and conformational flexibility: A circular dichroism and molecular dynamics simulation study. Computational and Structural Biotechnology Journal, 2020, 18, 1160-1172.	1.9	10
110	Molecular dynamics simulation of the homogeneous nucleation of UF6 molecules: Configurations and infrared spectra of the excited hot clusters. Journal of Chemical Physics, 2000, 112, 3812-3819.	1.2	9
111	MD simulation of clusterâ€“surface impacts for metallic phases: soft landing, droplet spreading and implantation. Computer Physics Communications, 2001, 141, 1-16.	3.0	9
112	Condensation on nanorods by molecular dynamics. Journal of Chemical Physics, 2016, 144, 244702.	1.2	9
113	A highly vectorised â€œlink-cellâ€•FORTRAN code for the DL_POLY molecular dynamics simulation package. Computer Physics Communications, 2000, 125, 167-192.	3.0	8
114	Accelerating Molecular Dynamics Simulations on PlayStation 3 Platform Using Virtual-GRAPE Programming Model. SIAM Journal of Scientific Computing, 2008, 30, 3108-3125.	1.3	8
115	Application of isotropic periodic sum method for 4-pentyl-4â€²-cyanobiphenyl liquid crystal. Molecular Simulation, 2015, 41, 927-935.	0.9	8
116	Critical test of beadâ€“spring model to resolve the scaling laws of polymer melts: a molecular dynamics study. Molecular Simulation, 2017, 43, 1196-1201.	0.9	8
117	Mechanism for H2 diffusion in sII hydrates by molecular dynamics simulations. Journal of Chemical Physics, 2020, 153, 054706.	1.2	8
118	Molecular dynamics simulations of the homogeneous nucleation of UF6 and SF6 molecules: Effects of the intramolecular vibrational relaxations on the nucleation rates. Journal of Chemical Physics, 1998, 109, 4492-4497.	1.2	7
119	GPUâ€accelerated computation of electron transfer. Journal of Computational Chemistry, 2012, 33, 2351-2356.	1.5	7
120	Cell size dependence of orientational order of uniaxial liquid crystals in flat slit. Molecular Simulation, 2008, 34, 761-773.	0.9	6
121	Multibaricâ€“Multithermal Ensemble Study of Liquidâ€“Solid Phase Transition in Lennard-Jones Particles. Journal of the Physical Society of Japan, 2012, 81, SA014.	0.7	6
122	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.	1.5	6
123	Analysis of crystal growth of methane hydrate using molecular dynamics simulation. Molecular Simulation, 2015, 41, 918-922.	0.9	6
124	Critical test of isotropic periodic sum techniques with group-based cut-off schemes. Scientific Reports, 2018, 8, 4185.	1.6	6
125	A biointerface effect on the self-assembly of ribonucleic acids: a possible mechanism of RNA polymerisation in the self-replication cycle. Nanoscale, 2020, 12, 6691-6698.	2.8	6
126	Molecular Mechanism of Vapor-Liquid Nucleation. Progress of Theoretical Physics Supplement, 2000, 138, 257-258.	0.2	5

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127	Two-Dimensional Supercritical Behavior of an Ethanol Monolayer:Â A Molecular Dynamics Study. Langmuir, 2005, 21, 10885-10894.	1.6	5
128	Molecular dynamics simulations of structure-H hydrates formed with methane and 3,3-dimethylpentane or 2,2-dimethylpentane. Molecular Simulation, 2007, 33, 65-69.	0.9	5
129	Overheads in Accelerating Molecular Dynamics Simulations with GPUs. , 2008, , .		5
130	Molecular dynamics study of ethanol solvated by water on the Pt (111) surface. Chemical Physics, 2012, 402, 41-47.	0.9	5
131	Molecular dynamics simulation of heterogeneous nucleation on nanotubes. RSC Advances, 2015, 5, 40953-40963.	1.7	5
132	Effects of temperature, concentration, and isomer on the hydration structure in monosaccharide solutions. Physical Chemistry Chemical Physics, 2017, 19, 15239-15246.	1.3	5
133	Effect of Central Longitudinal Dipole Interactions on Chiral Liquid-Crystal Phases. International Journal of Molecular Sciences, 2018, 19, 2715.	1.8	5
134	Detection of molecular behavior that characterizes systems using a deep learning approach. Nanoscale, 2019, 11, 10064-10071.	2.8	5
135	On effective radii of dodecahedral cages in semiclathrate hydrates for van der Waals and Platteeuw model. Fluid Phase Equilibria, 2021, 527, 112846.	1.4	5
136	Accelerating Molecular Dynamics Simulation Using Graphics Processing Unit. Bulletin of the Korean Chemical Society, 2010, 31, 3639-3643.	1.0	5
137	Nanoscale droplet vaporisation by molecular dynamics. Molecular Simulation, 2015, 41, 896-904.	0.9	4
138	A determination of liquidâ€“vapour interfacial properties for methanol using a linear-combination-based isotropic periodic sum. Molecular Simulation, 2015, 41, 795-800.	0.9	4
139	Replica exchange molecular simulation of Lennardâ€“Jones particles in a two-dimensional confined system. AIP Advances, 2017, 7, .	0.6	4
140	Heterogeneous cavitation and crystallisation with an impurity by molecular dynamics. Molecular Simulation, 2018, 44, 530-533.	0.9	4
141	Self-assembly of peptide amphiphiles by vapor pressure osmometry and dissipative particle dynamics. RSC Advances, 2018, 8, 26461-26468.	1.7	4
142	Molecular Dynamics Simulation of Ice Crystal Growth Inhibition by Hexadecyl-trimethyl-ammonium Bromide. Langmuir, 2018, 34, 9330-9335.	1.6	4
143	Separation of waterâ€“alcohol mixtures using carbon nanotubes under an electric field. Physical Chemistry Chemical Physics, 2019, 21, 15431-15438.	1.3	4
144	Ordering in clusters of uniaxial anisotropic particles during homogeneous nucleation and growth. Journal of Chemical Physics, 2019, 150, 054903.	1.2	4

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145	Phase Transitions and Hysteresis for a Simple Model Liquid Crystal by Replica-Exchange Monte Carlo Simulations. Molecules, 2021, 26, 1421.	1.7	4
146	Phase Equilibrium Calculation for Clathrate Hydrates Based on a Statistical Thermodynamics Model: An Attempt to Optimize the Kihara Parameters for Methane and Ethane. Japanese Journal of Applied Physics, 2007, 46, 5944-5950.	0.8	3
147	FAST QUASI DOUBLE-PRECISION METHOD WITH SINGLE-PRECISION HARDWARE TO ACCELERATE SCIENTIFIC APPLICATIONS. International Journal of Computational Methods, 2011, 08, 561-581.	0.8	3
148	Aspect ratio effect of nanorods on heterogeneous nucleation rates by molecular dynamics. Journal of Thermal Science and Technology, 2016, 11, JTST0044-JTST0044.	0.6	3
149	Structural determinants in the bulk heterojunction. Physical Chemistry Chemical Physics, 2018, 20, 5708-5720.	1.3	3
150	The influence of random number generation in dissipative particle dynamics simulations using a cryptographic hash function. PLoS ONE, 2021, 16, e0250593.	1.1	3
151	An analysis of natural convection using the thermal finite element discrete Boltzmann equation. Computers and Fluids, 2011, 40, 113-117.	1.3	2
152	Model of Abnormal Chromophore-Protein Interaction for E181K Rhodopsin Mutation: Computer Molecular Dynamics Study. The Open Biochemistry Journal, 2012, 6, 94-102.	0.3	2
153	Vibrational spectra of deuterated methane and water molecules in structure I clathrate hydrate fromab initioMD simulation. Molecular Simulation, 2015, 41, 813-817.	0.9	2
154	Instability of buried hydration sites increases protein subdomains fluctuations in the human prion protein by the pathogenic mutation T188R. AIP Advances, 2016, 6, .	0.6	2
155	A fast and accurate computational method for the linear-combination-based isotropic periodic sum. Scientific Reports, 2018, 8, 11880.	1.6	2
156	An Efficient Random Number Generation Method for Molecular Simulation. Journal of Chemical Information and Modeling, 2022, 62, 71-78.	2.5	2
157	Optimal Replica-Exchange Molecular Simulations in Combination with Evolution Strategies. Journal of Chemical Information and Modeling, 2022, 62, 6544-6552.	2.5	2
158	Microscopic Study of Nuclear â€œPastaâ€•by Quantum Molecular Dynamics. Progress of Theoretical Physics Supplement, 2002, 146, 638-639.	0.2	1
159	Molecular Dynamics Simulation of Cluster-Beam-Surface Impact Processes for Metallic Phases. Journal of Computational Methods in Sciences and Engineering, 2002, 2, 141-147.	0.1	1
160	Microscopic study of nuclear â€œpastaâ€• Quantum molecular dynamics approach. Nuclear Physics A, 2003, 718, 700-702.	0.6	1
161	Molecular dynamics simulation of time-irreversibility of stationary heat flux. Molecular Simulation, 2007, 33, 109-113.	0.9	1
162	Velocity auto-correlation function of ions and water molecules in different concentrations, anions and ion clusters. Molecular Simulation, 2015, 41, 840-844.	0.9	1

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163	GPU-accelerated replica exchange molecular simulation on solidâ€“liquid phase transition study of Lennard-Jones fluids. Molecular Simulation, 2015, 41, 874-880.	0.9	1
164	Structures of Water Molecules in Carbon Nanotubes Induced with Electric Fields and its Application for Water-Methanol Separation. Applied Mechanics and Materials, 2016, 842, 453-456.	0.2	1
165	Method To Implement Interaction Surfaces with Virtual Companion Particles for Molecular Dynamics Simulations. Journal of Chemical & Engineering Data, 2019, 64, 3693-3700.	1.0	1
166	Water molecules in CNTâ€“Si3N4 membrane: Properties and the separation effect for waterâ€“alcohol solution. Journal of Chemical Physics, 2021, 155, 104701.	1.2	1
167	Evaporation and condensation at a liquid methanol surface. Journal of Molecular Structure, 1994, 310, 161-168.	1.8	0
168	Nuclear Pasta Structure in Hot Neutron Stars. Symposium - International Astronomical Union, 2004, 218, 297-298.	0.1	0
169	1P117 Computational study of Aquaporin(Membrane proteins,Poster Presentations). Seibutsu Butsuri, 2007, 47, S52.	0.0	0
170	3P-105 Molecular Dynamics Simulations of Aquaporin(The 46th Annual Meeting of the Biophysical) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5	0.0	0
171	1A1448 Molecular Dynamics Simulations on Pressure Reversal of General Anesthesia in a Lipid Bilayer(Biol & Artifi memb 1: Structure & Property, Dynamics,The 49th Annual Meeting of the) Tj ETQq1 1 0.784314 rgBT /O	0.0	0
172	3PT155 Direct observations of flip-flops in membranes(The 50th Annual Meeting of the Biophysical) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5	0.0	0
173	1PT004 Mean Exit Time Analysis about Water Molecules around Membrane Surfaces(The 50th Annual) Tj ETQq1 1 0.784314 rgBT /Ov	0.0	0
174	Homogeneous connectivity of potential energy network in a solidlike state of water cluster. Journal of Chemical Physics, 2013, 138, 244301.	1.2	0
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