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	Natural quantum reservoir computing for temporal information processing. Scientific Reports, 2022, 12, 1353.	1.6	19
2	Efficient Monte Carlo Sampling for Molecular Systems Using Continuous Normalizing Flow. Journal of Chemical Theory and Computation, 2022, 18, 1395-1405.	2.3	0
3	An Efficient Random Number Generation Method for Molecular Simulation. Journal of Chemical Information and Modeling, 2022, 62, 71-78.	2.5	2
4	A stochastic Hamiltonian formulation applied to dissipative particle dynamics. Applied Mathematics and Computation, 2022, 426, 127126.	1.4	0
5	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
6	Optimal Replica-Exchange Molecular Simulations in Combination with Evolution Strategies. Journal of Chemical Information and Modeling, 2022, 62, 6544-6552.	2.5	2
7	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
8	Phase Transitions and Hysteresis for a Simple Model Liquid Crystal by Replica-Exchange Monte Carlo Simulations. Molecules, 2021, 26, 1421.	1.7	4
9	The influence of random number generation in dissipative particle dynamics simulations using a cryptographic hash function. PLoS ONE, 2021, 16, e0250593.	1.1	3
10	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
11	Mechanism for H2 diffusion in sII hydrates by molecular dynamics simulations. Journal of Chemical Physics, 2020, 153, 054706.	1.2	8
12	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
13	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
14	Dataflow programming for the analysis of molecular dynamics with AViS, an analysis and visualization software application. PLoS ONE, 2020, 15, e0231714.	1.1	0
15	Separation of waterâ€“alcohol mixtures using carbon nanotubes under an electric field. Physical Chemistry Chemical Physics, 2019, 21, 15431-15438.	1.3	4
16	Crystal Engineering of Bi₂WO₆ to Polar Aurivillius-Phase Oxyhalides. Journal of Physical Chemistry C, 2019, 123, 29155-29161.	1.5	12
17	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
18	Detection of molecular behavior that characterizes systems using a deep learning approach. Nanoscale, 2019, 11, 10064-10071.	2.8	5

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19	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
20	Molecular Dynamic Simulations to Probe Water Permeation Pathways of GPCRs. Methods in Molecular Biology, 2019, 1947, 21-30.	0.4	0
21	Ordering in clusters of uniaxial anisotropic particles during homogeneous nucleation and growth. Journal of Chemical Physics, 2019, 150, 054903.	1.2	4
22	Selectivity of Carbon Nanotubes under An Electric Field on Transferring Water â€“ Alcohol Mixtures. IOP Conference Series: Materials Science and Engineering, 2019, 494, 012099.	0.3	0
23	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
24	Structural determinants in the bulk heterojunction. Physical Chemistry Chemical Physics, 2018, 20, 5708-5720.	1.3	3
25	Detection of Anomalous Dynamics for a Single Water Molecule. Journal of Chemical Theory and Computation, 2018, 14, 1177-1185.	2.3	0
26	Critical test of isotropic periodic sum techniques with group-based cut-off schemes. Scientific Reports, 2018, 8, 4185.	1.6	6
27	Heterogeneous cavitation and crystallisation with an impurity by molecular dynamics. Molecular Simulation, 2018, 44, 530-533.	0.9	4
28	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
29	Recent Advances in Clathrate Hydrates Research using Molecular Simulations. Review of High Pressure Science and Technology/Koatsuryoku No Kagaku To Gijutsu, 2018, 28, 102-112.	0.1	0
30	Effect of Central Longitudinal Dipole Interactions on Chiral Liquid-Crystal Phases. International Journal of Molecular Sciences, 2018, 19, 2715.	1.8	5
31	Kinetic analysis of homogeneous droplet nucleation using large-scale molecular dynamics simulations. Journal of Chemical Physics, 2018, 149, 044504.	1.2	20
32	Self-assembly of peptide amphiphiles by vapor pressure osmometry and dissipative particle dynamics. RSC Advances, 2018, 8, 26461-26468.	1.7	4
33	Molecular Dynamics Simulation of Ice Crystal Growth Inhibition by Hexadecyl-trimethyl-ammonium Bromide. Langmuir, 2018, 34, 9330-9335.	1.6	4
34	Oxygen vacancy-originated highly active electrocatalysts for the oxygen evolution reaction. Journal of Materials Chemistry A, 2018, 6, 15102-15109.	5.2	67
35	A fast and accurate computational method for the linear-combination-based isotropic periodic sum. Scientific Reports, 2018, 8, 11880.	1.6	2
36	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

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37	Dynamic interactions between a membrane binding protein and lipids induce fluctuating diffusivity. Science Advances, 2017, 3, e1601871.	4.7	59
38	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
39	Replica exchange molecular simulation of Lennardâ€“Jones particles in a two-dimensional confined system. AIP Advances, 2017, 7, .	0.6	4
40	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
41	Effects of temperature, concentration, and isomer on the hydration structure in monosaccharide solutions. Physical Chemistry Chemical Physics, 2017, 19, 15239-15246.	1.3	5
42	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
43	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
44	Onset of static and dynamic universality among molecular models of polymers. Scientific Reports, 2017, 7, 12379.	1.6	15
45	Molecular Dynamics Simulation of Water Nanodroplet Bounce Back from Flat and Nanopillared Surface. Langmuir, 2017, 33, 10184-10192.	1.6	40
46	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
47	Origin of the blueshift of water molecules at interfaces of hydrophilic cyclic compounds. Science Advances, 2017, 3, e1701400.	4.7	22
48	Water Molecules in a Carbon Nanotube under an Applied Electric Field at Various Temperatures and Pressures. Water (Switzerland), 2017, 9, 473.	1.2	29
49	Molecular Dynamics Simulations for Resolving Scaling Laws of Polyethylene Melts. Polymers, 2017, 9, 24.	2.0	25
50	Water permeation through the internal water pathway in activated GPCR rhodopsin. PLoS ONE, 2017, 12, e0176876.	1.1	14
51	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
52	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
53	Condensation on nanorods by molecular dynamics. Journal of Chemical Physics, 2016, 144, 244702.	1.2	9
54	Suppression of lattice thermal conductivity by mass-conserving cation mutation in multi-component semiconductors. APL Materials, 2016, 4, 104809.	2.2	12

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55	Interactions of Pleckstrin Homology Domains with Membranes: Adding Back the Bilayer via High-Throughput Molecular Dynamics. Structure, 2016, 24, 1421-1431.	1.6	68
56	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
57	Separation of waterâ€“ethanol solutions with carbon nanotubes and electric fields. Physical Chemistry Chemical Physics, 2016, 18, 33310-33319.	1.3	33
58	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
59	Anomalous Dynamics of a Lipid Recognition Protein on a Membrane Surface. Scientific Reports, 2016, 5, 18245.	1.6	38
60	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
61	Cage occupancy of methane hydrates from Gibbs ensemble Monte Carlo simulations. Fluid Phase Equilibria, 2016, 413, 242-248.	1.4	36
62	Analysis of three-phase equilibrium points for methane hydrate/water/methane systems by NVT molecular dynamics simulation. The Proceedings of the Thermal Engineering Conference, 2016, 2016, I222.	0.0	0
63	Molecular dynamics study on the dynamics of water molecules in hydration shell of monosaccharides. The Proceedings of the Thermal Engineering Conference, 2016, 2016, G221.	0.0	0
64	Origin of 1/f noise in hydration dynamics on lipid membrane surfaces. Scientific Reports, 2015, 5, 8876.	1.6	14
65	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
66	Anomalous Diffusion of Water Molecules on Cell Membranes Investigated by Using Molecular Dynamics Simulations. Seibutsu Butsuri, 2015, 55, 242-245.	0.0	0
67	Analysis of crystal growth of methane hydrate using molecular dynamics simulation. Molecular Simulation, 2015, 41, 918-922.	0.9	6
68	Nanoscale droplet vaporisation by molecular dynamics. Molecular Simulation, 2015, 41, 896-904.	0.9	4
69	Nucleation rate analysis of methane hydrate from molecular dynamics simulations. Faraday Discussions, 2015, 179, 463-474.	1.6	57
70	Waterâ€“methanol separation with carbon nanotubes and electric fields. Nanoscale, 2015, 7, 12659-12665.	2.8	33
71	Molecular dynamics simulation of heterogeneous nucleation on nanotubes. RSC Advances, 2015, 5, 40953-40963.	1.7	5
72	A molecular dynamics study of guestâ€“host hydrogen bonding in alcohol clathrate hydrates. Physical Chemistry Chemical Physics, 2015, 17, 12639-12647.	1.3	24

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73	Application of isotropic periodic sum method for 4-pentyl-4â€²-cyanobiphenyl liquid crystal. Molecular Simulation, 2015, 41, 927-935.	0.9	8
74	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
75	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
76	Structures of water molecules in carbon nanotubes under electric fields. Journal of Chemical Physics, 2015, 142, 124701.	1.2	45
77	Approaches for Controlling the Temperature and Pressure Range in Generalized NPT Ensembles. Journal of Chemical Theory and Computation, 2015, 11, 4370-4376.	2.3	0
78	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
79	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
80	Water Confined in the Local Field of Ions. ChemPhysChem, 2014, 15, 4077-4086.	1.0	40
81	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
82	Observation of Interstitial Molecular Hydrogen in Clathrate Hydrates. Angewandte Chemie - International Edition, 2014, 53, 10710-10713.	7.2	14
83	<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:m of amino acids regulate water transportation in aquaporin 1. Physical Review E, 2014, 89, 022718.	2.4	27
84	Poisson property of the occurrence of flip-flops in a model membrane. Journal of Chemical Physics, 2014, 140, 064901.	1.2	15
85	From kesterite to stannite photovoltaics: Stability and band gaps of the Cu2(Zn,Fe)SnS4 alloy. Applied Physics Letters, 2014, 104, .	1.5	76
86	Bipolaron Formation Induced by Oxygen Vacancy at Rutile TiO₂(110) Surfaces. Journal of Physical Chemistry C, 2014, 118, 9429-9435.	1.5	31
87	1/F Fluctuations of Amino Acids Generate Non-Poisson Water Transportation in AQP1. Biophysical Journal, 2014, 106, 559a.	0.2	0
88	Origin of subdiffusion of water molecules on cell membrane surfaces. Scientific Reports, 2014, 4, 4720.	1.6	84
89	B224 1/f fluctuation of number of water molecules on lipid bilayers. The Proceedings of the Thermal Engineering Conference, 2014, 2014, _B224-1_-_B224-2_.	0.0	0
90	Phase diagrams of confined solutions of dimyristoylphosphatidylcholine (DMPC) lipid and cholesterol in nanotubes. Microfluidics and Nanofluidics, 2013, 14, 995-1010.	1.0	11

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91	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
92	Dynamic interactions of cations, water and lipids and influence on membrane fluidity. Journal of Membrane Science, 2013, 435, 130-136.	4.1	20
93	A vesicle cell under collision with a Janus or homogeneous nanoparticle: translocation dynamics and late-stage morphology. Nanoscale, 2013, 5, 9089.	2.8	50
94	Water proton configurations in structures I, II, and H clathrate hydrate unit cells. Journal of Chemical Physics, 2013, 138, 124504.	1.2	193
95	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
96	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
97	Petascale turbulence simulation using a highly parallel fast multipole method on GPUs. Computer Physics Communications, 2013, 184, 445-455.	3.0	51
98	Homogeneous connectivity of potential energy network in a solidlike state of water cluster. Journal of Chemical Physics, 2013, 138, 244301.	1.2	0
99	Power-law trapping of water molecules on the lipid-membrane surface induces water retardation. Physical Review E, 2013, 87, 052715.	0.8	23
100	2P130 Water behavior in buried hydration sites of human cellular prion protein and pathogenic mutation T188R(07. Water & Hydration & Electrolyte,Poster). Seibutsu Butsuri, 2013, 53, S180.	0.0	0
101	2P131 Aging of water molecules on cell membrane surfaces(07. Water & Hydration &) Tj ETQq1 1 0.784314 rgBT /Overlock	0.0	0
102	G141 Molecular dynamics simulation of methane hydrate growth on water/methane interface. The Proceedings of the Thermal Engineering Conference, 2013, 2013, 223-224.	0.0	0
103	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
104	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
105	3PT155 Direct observations of flip-flops in membranes(The 50th Annual Meeting of the Biophysical) Tj ETQq1 1 0.784314 rgBT /Overl	0.0	0
106	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
107	GPUâ€accelerated computation of electron transfer. Journal of Computational Chemistry, 2012, 33, 2351-2356.	1.5	7
108	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

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109	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
110	Nanochannel with Uniform and Janus Surfaces: Shear Thinning and Thickening in Surfactant Solution. Langmuir, 2012, 28, 2866-2872.	1.6	23
111	Nanoparticle Growth Analysis by Molecular Dynamics: Cubic Seed. Journal of Physical Chemistry B, 2012, 116, 14637-14649.	1.2	20
112	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
113	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
114	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
115	1PT004 Mean Exit Time Analysis about Water Molecules around Membrane Surfaces(The 50th Annual) Tj ETQq1 1 0.784314 rgBT /Ov	0.0	0
116	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
117	Molecular dynamics study of ethanol solvated by water on the Pt (111) surface. Chemical Physics, 2012, 402, 41-47.	0.9	5
118	Size-Dependent Phase Changes in Water Clusters. Journal of Chemical Theory and Computation, 2011, 7, 3083-3087.	2.3	19
119	Thermodynamic properties of methane/water interface predicted by molecular dynamics simulations. Journal of Chemical Physics, 2011, 134, 144702.	1.2	55
120	Nanoparticle Growth Analysis by Molecular Dynamics: Spherical Seed. Journal of Physical Chemistry B, 2011, 115, 10631-10645.	1.2	28
121	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
122	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
123	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 /Ov		
124	An analysis of natural convection using the thermal finite element discrete Boltzmann equation. Computers and Fluids, 2011, 40, 113-117.	1.3	2
125	Non-Gaussian Fluctuations Resulting from Power-Law Trapping in a Lipid Bilayer. Physical Review Letters, 2011, 107, 178103.	2.9	87
126	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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127	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
128	Molecular dynamics simulations of vapor/liquid coexistence using the nonpolarizable water models. Journal of Chemical Physics, 2011, 134, 124708.	1.2	60
129	Energy science of clathrate hydrates: Simulation-based advances. MRS Bulletin, 2011, 36, 205-210.	1.7	17
130	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
131	Phase diagram of Lennard-Jones fluid confined in slit pores. Chemical Physics Letters, 2010, 490, 165-171.	1.2	29
132	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
133	Asymmetric Brownian Motor Driven by Bubble Formation in a Hydrophobic Channel. ACS Nano, 2010, 4, 5905-5913.	7.3	14
134	Molecular dynamics simulations of ureaâ€“water binary droplets on flat and pillared hydrophobic surfaces. Faraday Discussions, 2010, 146, 185.	1.6	20
135	Accelerating Molecular Dynamics Simulation Using Graphics Processing Unit. Bulletin of the Korean Chemical Society, 2010, 31, 3639-3643.	1.0	5
136	Formation of Nuclear â€œPastaâ€•in Supernovae. Physical Review Letters, 2009, 103, 121101.	2.9	69
137	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
138	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
139	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
140	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
141	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
142	Self-Assembly of Surfactants and Polymorphic Transition in Nanotubes. Journal of the American Chemical Society, 2008, 130, 7916-7920.	6.6	87
143	Overheads in Accelerating Molecular Dynamics Simulations with GPUs. , 2008, , .		5
144	Cell size dependence of orientational order of uniaxial liquid crystals in flat slit. Molecular Simulation, 2008, 34, 761-773.	0.9	6

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145	Phase diagram of nuclear â€œpastaâ€•and its uncertainties in supernova cores. Physical Review C, 2008, 77, .	1.1	77
146	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
147	Extended study of molecular dynamics simulation of homogeneous vapor-liquid nucleation of water. Journal of Chemical Physics, 2007, 127, 214507.	1.2	49
148	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
149	Spontaneous self-assembly process for threadlike micelles. Journal of Chemical Physics, 2007, 126, 244905.	1.2	47
150	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
151	Molecular dynamics simulation of time-irreversibility of stationary heat flux. Molecular Simulation, 2007, 33, 109-113.	0.9	1
152	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
153	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
154	Impact of nuclear â€œpastaâ€•on neutrino transport in collapsing stellar cores. Physical Review C, 2007, 75, .	1.1	44
155	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
156	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
157	1P117 Computational study of Aquaporin(Membrane proteins,Poster Presentations). Seibutsu Butsuri, 2007, 47, S52.	0.0	0
158	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
159	Free-energy calculation of structure-H hydrates. Journal of Chemical Physics, 2006, 124, 024510.	1.2	52
160	Hydrogen-Bonded Clusters on the Vapor/Ethanol-Aqueous-Solution Interface. Journal of Physical Chemistry B, 2006, 110, 23264-23273.	1.2	18
161	Large-scale molecular-dynamics simulation of nanoscale hydrophobic interaction and nanobubble formation. Journal of Chemical Physics, 2005, 123, 204707.	1.2	46
162	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

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163	Two-Dimensional Supercritical Behavior of an Ethanol Monolayer:Â A Molecular Dynamics Study. Langmuir, 2005, 21, 10885-10894.	1.6	5
164	C141 Variation of microscopic structure of ethanol/cyclohexane binary liquid with molar fraction and molecular description of diffusion coefficient of ethanol. The Proceedings of the Thermal Engineering Conference, 2005, 2005, 117-118.	0.0	0
165	2805 Molecular dynamics study of ethanol macrocluster formation on silica surfaces. The Proceedings of the Computational Mechanics Conference, 2005, 2005.18, 43-44.	0.0	0
166	Nuclear Pasta Structure in Hot Neutron Stars. Symposium - International Astronomical Union, 2004, 218, 297-298.	0.1	0
167	Phases of hot nuclear matter at subnuclear densities. Physical Review C, 2004, 69, .	1.1	52
168	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
169	Hardware accelerator for molecular dynamics: MDGRAPE-2. Computer Physics Communications, 2003, 155, 115-131.	3.0	60
170	Microscopic study of nuclear â€œpastaâ€• Quantum molecular dynamics approach. Nuclear Physics A, 2003, 718, 700-702.	0.6	1
171	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
172	Large scale molecular dynamics simulation of nucleation in supercooled NaCl. Journal of Chemical Physics, 2003, 119, 11298-11305.	1.2	32
173	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
174	Structure of cold nuclear matter at subnuclear densities by quantum molecular dynamics. Physical Review C, 2003, 68, .	1.1	80
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