Noriyuki Yoshii

List of Publications by Year
in descending order

37 papers	758 citations	687363 13 h-index	526287 27 g-index
37 all docs	37 docs citations	37 times ranked	707 citing authors

#	Article	IF	Citations
1	A molecular dynamics study of sub- and supercritical water using a polarizable potential model. Journal of Chemical Physics, 1998, 109, 4873-4884.	3.0	101
2	MODYLAS: A Highly Parallelized General-Purpose Molecular Dynamics Simulation Program for Large-Scale Systems with Long-Range Forces Calculated by Fast Multipole Method (FMM) and Highly Scalable Fine-Grained New Parallel Processing Algorithms. Journal of Chemical Theory and Computation, 2013, 9, 3201-3209.	5.3	85
3	A molecular dynamics study of free energy of micelle formation for sodium dodecyl sulfate in water and its size distribution. Journal of Chemical Physics, 2006, 124, 184901.	3.0	73
4	A molecular dynamics study of dielectric constant of water from ambient to sub- and supercritical conditions using a fluctuating-charge potential model. Chemical Physics Letters, 2001, 345, 195-200.	2.6	69
5	A large-scale and long-time molecular dynamics study of supercritical Lennard-Jones fluid. An analysis of high temperature clusters. Journal of Chemical Physics, 1997, 107, 2020-2033.	3.0	51
6	A molecular dynamics study of structural stability of spherical SDS micelle as a function of its size. Chemical Physics Letters, 2006, 425, 58-61.	2.6	46
7	All-Atom Molecular Dynamics Study of a Spherical Micelle Composed of N-Acetylated Poly(ethylene) Tj ETQq1 1 0.784314 rgBT /Overlo Systems for Cancer. Journal of Physical Chemistry B, 2009, 113, 15181-15188.	2.6	34
8	A molecular dynamics study of surface structure of spherical SDS micelles. Chemical Physics Letters, 2006, 426, 66-70.	2.6	29
9	A molecular-dynamics study of the equation of state of water using a fluctuating-charge model. Chemical Physics Letters, 2000, 317, 414-420.	2.6	25
10	Density Fluctuation and Hydrogen-Bonded Clusters in Supercritical Water. A Molecular Dynamics Analysis Using a Polarizable Potential Model. Bulletin of the Chemical Society of Japan, 1999, 72, 151-162.	3.2	22
11	Drug binding and mobility relating to the thermal fluctuation in fluid lipid membranes. Journal of Chemical Physics, 2008, 129, 215102.	3.0	20
12	Free energy of water permeation into hydrophobic core of sodium dodecyl sulfate micelle by molecular dynamics calculation. Journal of Chemical Physics, 2007, 126, 096101.	3.0	19
13	Molecular dynamics study of the formation mechanisms of ionic SDS and nonionic C12E8 micelles and n-dodecane droplets. Chemical Physics Letters, 2016, 646, 36-40.	2.6	18
14	Molecular dynamics study of structure of clusters in supercritical Lennardâ€“Jones fluid. Fluid Phase Equilibria, 1998, 144, 225-232.	2.5	13
15	A large-scale molecular dynamics study of dynamic structure factor and dispersion relation of acoustic mode in liquid and supercritical water. Fluid Phase Equilibria, 2004, 226, 345-350.	2.5	13
16	Electrostatic potential gap at the interface between triethylamine and water phases studied by molecular dynamics simulation. Chemical Physics Letters, 2007, 448, 70-74.	2.6	13
17	Kinetics of membrane binding and dissociation of 5-fluorouracil by pulsed-field-gradient 19F NMR. Chemical Physics Letters, 2009, 474, 357-361.	2.6	12
18	Molecular dynamics study of the structure of anionic SDS, cationic DTAC, zwitterionic DDAO, and nonionic C12E8 spherical micelles in solution. Journal of Molecular Liquids, 2016, 217, 99-102.	4.9	11

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19	Molecular dynamics study of the potential of mean force of SDS aggregates. Journal of Chemical Physics, 2017, 147, 084903.	3.0	11
20	A molecular dynamics study of local pressures and interfacial tensions of SDS micelles and dodecane droplets in water. Journal of Chemical Physics, 2016, 144, 224701.	3.0	10
21	Binding of Hydrophobic Fluorinated Bisphenol A to Large Unilamellar Vesicles of Egg Phosphatidylcholine. Journal of Physical Chemistry B, 2011, 115, 11074-11080.	2.6	8
22	A molecular dynamics study of the breathing and deforming modes of the spherical ionic SDS and nonionic C12E8 micelles. Journal of Chemical Physics, 2016, 144, 034903.	3.0	8
23	Evaluation of atomic pressure in the multiple timeâ€step integration algorithm. Journal of Computational Chemistry, 2017, 38, 704-713.	3.3	8
24	Lateral diffusion of lipids separated from rotational and translational diffusion of a fluid large unilamellar vesicle. Colloids and Surfaces B: Biointerfaces, 2013, 106, 22-27.	5.0	7
25	Molecular dynamics study of the aggregation rate for zwitterionic dodecyldimethylamine oxide and cationic dodecyltrimethylammonium chloride micelles. Molecular Simulation, 2017, 43, 1331-1337.	2.0	7
26	Algorithm to minimize <scp>MPI</scp> communications in the parallelized fast multipole method combined with molecular dynamics calculations. Journal of Computational Chemistry, 2021, 42, 1073-1087.	3.3	7
27	Extension of the fast multipole method for the rectangular cells with an anisotropic partition tree structure. Journal of Computational Chemistry, 2020, 41, 1353-1367.	3.3	6
28	Spherical harmonics analysis of surface density fluctuations of spherical ionic SDS and nonionic C12E8 micelles: A molecular dynamics study. Journal of Chemical Physics, 2017, 147, 034906.	3.0	5
29	Exact long-range Coulombic energy calculation for net charged systems neutralized by uniformly distributed background charge using fast multipole method and its application to efficient free energy calculation. Journal of Chemical Physics, 2020, 152, 244115.	3.0	5
30	Fast multipole method for threeâ€dimensional systems with periodic boundary condition in two directions. Journal of Computational Chemistry, 2020, 41, 940-948.	3.3	5
31	MODYLAS: A highly parallelized generalâ€purpose molecular dynamics simulation program. International Journal of Quantum Chemistry, 2015, 115, 342-348.	2.0	4
32	A thread-level parallelization of pairwise additive potential and force calculations suitable for current many-core architectures. Journal of Supercomputing, 2018, 74, 2449-2469.	3.6	4
33	Molecular dynamics study of solubilization of cyclohexane, benzene, and phenol into mixed micelles composed of sodium dodecyl sulfate and octaethylene glycol monododecyl ether. Journal of Computational Chemistry, 2019, 40, 2722-2729.	3.3	3
34	Prediction of Thermal Properties and Effect of OH Substituent for Poly(vinyl alcohol)s by Molecular Dynamics Calculations. Japanese Journal of Applied Physics, 2004, 43, 5676-5681.	1.5	2
35	A molecular analysis of the vibrational energy relaxation mechanism of the CNâ¯ ion in water based upon path integral influence functional theory combined with a dipole expansion of the soluteâ€“solvent interaction. Journal of Molecular Liquids, 2007, 134, 34-39.	4.9	2
36	Pressure tensor for electrostatic interaction calculated by fast multipole method with periodic boundary condition. Journal of Computational Chemistry, 2018, 39, 1192-1199.	3.3	2

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37	Dynamics in Fluids. Computer Simulation of Supercritical Water and Aqueous Solutions.. Review of High Pressure Science and Technology/Koatsuryoku No Kagaku To Gijutsu, 2000, 10, 275-282.	0.0	0