

Noriyuki Yoshii

List of Publications by Year in descending order

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687363

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#	ARTICLE	IF	CITATIONS
1	Algorithm to minimize <sc>MPI</sc> communications in the parallelized fast multipole method combined with molecular dynamics calculations. <i>Journal of Computational Chemistry</i> , 2021, 42, 1073-1087.	3.3	7
2	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. <i>Journal of Chemical Physics</i> , 2020, 152, 244115.	3.0	5
3	Extension of the fast multipole method for the rectangular cells with an anisotropic partition tree structure. <i>Journal of Computational Chemistry</i> , 2020, 41, 1353-1367.	3.3	6
4	Fast multipole method for three-dimensional systems with periodic boundary condition in two directions. <i>Journal of Computational Chemistry</i> , 2020, 41, 940-948.	3.3	5
5	Molecular dynamics study of solubilization of cyclohexane, benzene, and phenol into mixed micelles composed of sodium dodecyl sulfate and octaethylene glycol monododecyl ether. <i>Journal of Computational Chemistry</i> , 2019, 40, 2722-2729.	3.3	3
6	Pressure tensor for electrostatic interaction calculated by fast multipole method with periodic boundary condition. <i>Journal of Computational Chemistry</i> , 2018, 39, 1192-1199.	3.3	2
7	A thread-level parallelization of pairwise additive potential and force calculations suitable for current many-core architectures. <i>Journal of Supercomputing</i> , 2018, 74, 2449-2469.	3.6	4
8	Evaluation of atomic pressure in the multiple time-step integration algorithm. <i>Journal of Computational Chemistry</i> , 2017, 38, 704-713.	3.3	8
9	Molecular dynamics study of the potential of mean force of SDS aggregates. <i>Journal of Chemical Physics</i> , 2017, 147, 084903.	3.0	11
10	Spherical harmonics analysis of surface density fluctuations of spherical ionic SDS and nonionic C12E8 micelles: A molecular dynamics study. <i>Journal of Chemical Physics</i> , 2017, 147, 034906.	3.0	5
11	Molecular dynamics study of the aggregation rate for zwitterionic dodecyl dimethylamine oxide and cationic dodecyl trimethylammonium chloride micelles. <i>Molecular Simulation</i> , 2017, 43, 1331-1337.	2.0	7
12	A molecular dynamics study of local pressures and interfacial tensions of SDS micelles and dodecane droplets in water. <i>Journal of Chemical Physics</i> , 2016, 144, 224701.	3.0	10
13	A molecular dynamics study of the breathing and deforming modes of the spherical ionic SDS and nonionic C12E8 micelles. <i>Journal of Chemical Physics</i> , 2016, 144, 034903.	3.0	8
14	Molecular dynamics study of the structure of anionic SDS, cationic DTAC, zwitterionic DDAO, and nonionic C12E8 spherical micelles in solution. <i>Journal of Molecular Liquids</i> , 2016, 217, 99-102.	4.9	11
15	Molecular dynamics study of the formation mechanisms of ionic SDS and nonionic C12E8 micelles and n-dodecane droplets. <i>Chemical Physics Letters</i> , 2016, 646, 36-40.	2.6	18
16	MODYLAS: A highly parallelized general-purpose molecular dynamics simulation program. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 342-348.	2.0	4
17	Lateral diffusion of lipids separated from rotational and translational diffusion of a fluid large unilamellar vesicle. <i>Colloids and Surfaces B: Biointerfaces</i> , 2013, 106, 22-27.	5.0	7
18	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. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3201-3209.	5.3	85

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19	Binding of Hydrophobic Fluorinated Bisphenol A to Large Unilamellar Vesicles of Egg Phosphatidylcholine. <i>Journal of Physical Chemistry B</i> , 2011, 115, 11074-11080.	2.6	8
20	Kinetics of membrane binding and dissociation of 5-fluorouracil by pulsed-field-gradient 19F NMR. <i>Chemical Physics Letters</i> , 2009, 474, 357-361.	2.6	12
21	All-Atom Molecular Dynamics Study of a Spherical Micelle Composed of N-Acetylated Poly(ethylene) Tj ETQq1 1 0.784314 rgBT /Overl Systems for Cancer. <i>Journal of Physical Chemistry B</i> , 2009, 113, 15181-15188.	2.6	34
22	Drug binding and mobility relating to the thermal fluctuation in fluid lipid membranes. <i>Journal of Chemical Physics</i> , 2008, 129, 215102.	3.0	20
23	Free energy of water permeation into hydrophobic core of sodium dodecyl sulfate micelle by molecular dynamics calculation. <i>Journal of Chemical Physics</i> , 2007, 126, 096101.	3.0	19
24	Electrostatic potential gap at the interface between triethylamine and water phases studied by molecular dynamics simulation. <i>Chemical Physics Letters</i> , 2007, 448, 70-74.	2.6	13
25	A molecular analysis of the vibrational energy relaxation mechanism of the CN ⁺ ion in water based upon path integral influence functional theory combined with a dipole expansion of the solute-solvent interaction. <i>Journal of Molecular Liquids</i> , 2007, 134, 34-39.	4.9	2
26	A molecular dynamics study of free energy of micelle formation for sodium dodecyl sulfate in water and its size distribution. <i>Journal of Chemical Physics</i> , 2006, 124, 184901.	3.0	73
27	A molecular dynamics study of structural stability of spherical SDS micelle as a function of its size. <i>Chemical Physics Letters</i> , 2006, 425, 58-61.	2.6	46
28	A molecular dynamics study of surface structure of spherical SDS micelles. <i>Chemical Physics Letters</i> , 2006, 426, 66-70.	2.6	29
29	Prediction of Thermal Properties and Effect of OH Substituent for Poly(vinyl alcohol)s by Molecular Dynamics Calculations. <i>Japanese Journal of Applied Physics</i> , 2004, 43, 5676-5681.	1.5	2
30	A large-scale molecular dynamics study of dynamic structure factor and dispersion relation of acoustic mode in liquid and supercritical water. <i>Fluid Phase Equilibria</i> , 2004, 226, 345-350.	2.5	13
31	A molecular dynamics study of dielectric constant of water from ambient to sub- and supercritical conditions using a fluctuating-charge potential model. <i>Chemical Physics Letters</i> , 2001, 345, 195-200.	2.6	69
32	A molecular-dynamics study of the equation of state of water using a fluctuating-charge model. <i>Chemical Physics Letters</i> , 2000, 317, 414-420.	2.6	25
33	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
34	Density Fluctuation and Hydrogen-Bonded Clusters in Supercritical Water. A Molecular Dynamics Analysis Using a Polarizable Potential Model. <i>Bulletin of the Chemical Society of Japan</i> , 1999, 72, 151-162.	3.2	22
35	A molecular dynamics study of sub- and supercritical water using a polarizable potential model. <i>Journal of Chemical Physics</i> , 1998, 109, 4873-4884.	3.0	101
36	Molecular dynamics study of structure of clusters in supercritical Lennard-Jones fluid. <i>Fluid Phase Equilibria</i> , 1998, 144, 225-232.	2.5	13

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37	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