

# Tatsuhiko Miyata

## List of Publications by Year in descending order

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Version: 2024-02-01

28  
papers

495  
citations

623734

14  
h-index

677142

22  
g-index

29  
all docs

29  
docs citations

29  
times ranked

459  
citing authors

#	ARTICLE	IF	CITATIONS
1	Combination of molecular dynamics method and 3D-RISM theory for conformational sampling of large flexible molecules in solution. <i>Journal of Computational Chemistry</i> , 2008, 29, 871-882.	3.3	73
2	Evaluation of pore size distribution in boundary region of micropore and mesopore using gas adsorption method. <i>Journal of Colloid and Interface Science</i> , 2003, 262, 116-125.	9.4	39
3	Molecular Approach To Understand the Tacticity Effects on the Hydrophilicity of Poly(N-isopropylacrylamide): Solubility of Dimer Model Compounds in Water. <i>Journal of Physical Chemistry B</i> , 2010, 114, 13312-13318.	2.6	37
4	Free energy calculation using molecular dynamics simulation combined with the three dimensional reference interaction site model theory. I. Free energy perturbation and thermodynamic integration along a coupling parameter. <i>Journal of Chemical Physics</i> , 2010, 133, 044114.	3.0	36
5	TiO <sub>2</sub> -montmorillonite composites via supercritical intercalation Electronic supplementary information (ESI) available: Figs. S1 and S2: powder XRD patterns. See <a href="http://www.rsc.org/suppdata/cc/b2/b202589b/">http://www.rsc.org/suppdata/cc/b2/b202589b/</a> . <i>Chemical Communications</i> , 2002, , 1526-1527.	4.1	34
6	Systematic Docking Study of the Carbohydrate Binding Module Protein of Cel7A with the Cellulose I <sub>1</sub> Crystal Model. <i>Journal of Physical Chemistry B</i> , 2010, 114, 49-58.	2.6	31
7	Thermodynamic significance to correct the location of first rising region in radial distribution function approximately estimated from Ornstein-Zernike integral equation theory for Lennard-Jones fluids. <i>Journal of Molecular Liquids</i> , 2016, 217, 75-82.	4.9	25
8	Synthesis of titania-pillared montmorillonite via intercalation of titanium alkoxide dissolved in supercritical carbon dioxide. <i>Journal of Materials Chemistry</i> , 2004, 14, 2763.	6.7	23
9	Accuracy of solvation free energy calculated by hypernetted chain and Kovalenko-Hirata approximations for two-component system of Lennard-Jones liquid. <i>Chemical Physics Letters</i> , 2014, 604, 122-126.	2.6	23
10	Free energy calculation using molecular dynamics simulation combined with the three-dimensional reference interaction site model theory. II. Thermodynamic integration along a spatial reaction coordinate. <i>Journal of Chemical Physics</i> , 2011, 134, 044127.	3.0	21
11	A pressure consistent bridge correction of Kovalenko-Hirata closure in Ornstein-Zernike theory for Lennard-Jones fluids by apparently adjusting sigma parameter. <i>AIP Advances</i> , 2016, 6, .	1.3	19
12	Brownian Dynamics Simulation Study of Self-Diffusion of a Charged Particle in Swollen Counter-Charged Hydrogel Modeled as Cubic Lattice.. <i>Journal of Chemical Engineering of Japan</i> , 2002, 35, 640-648.	0.6	18
13	Correction of Kovalenko-Hirata closure in Ornstein-Zernike integral equation theory for Lennard-Jones fluids. <i>Journal of Molecular Liquids</i> , 2017, 245, 2-10.	4.9	17
14	A Parameterization of Empirical Sigma Enlarging Bridge Correction of Kovalenko-Hirata Closure in Ornstein-Zernike Theory for Lennard-Jones Fluids. <i>Bulletin of the Chemical Society of Japan</i> , 2017, 90, 1095-1104.	3.2	16
15	Performance of Kobryn-Gusarov-Kovalenko closure from a thermodynamic viewpoint for one-component Lennard-Jones fluids. <i>Chemical Physics Letters</i> , 2018, 700, 88-95.	2.6	14
16	Accuracy of temperature-derivative of radial distribution function calculated under approximations in Ornstein-Zernike theory for one-component Lennard-Jones fluid. <i>Chemical Physics Letters</i> , 2016, 658, 224-229.	2.6	11
17	A study on the transferability of the sigma enlarging bridge function for an accurate evaluation of solvation free energy: The case of homonuclear Lennard-Jones diatomic solute solvated in a Lennard-Jones monatomic solvent. <i>AIP Advances</i> , 2019, 9, .	1.3	9
18	Prediction of cellulose nanotube models through density functional theory calculations. <i>Cellulose</i> , 2014, 21, 87-95.	4.9	7

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19	An assessment of the sigma enlarging bridge function for a Lennard-Jones solution using a solvent-solvent correlation function obtained from molecular dynamics simulation. <i>Journal of Molecular Liquids</i> , 2019, 290, 111167.	4.9	7
20	Sigma enlarging bridge function for heteronuclear Lennard-Jones diatomic solute solvated in a Lennard-Jones monatomic solvent in terms of the parameter transferability. <i>Chemical Physics Letters</i> , 2020, 755, 137777.	2.6	7
21	Brownian Dynamics Simulation of Self-Diffusion of Ionic Large Solute Molecule in Modeled Polyelectrolyte Gel. <i>Journal of the Physical Society of Japan</i> , 2012, 81, SA010.	1.6	6
22	Molecular dynamics simulations of theoretical cellulose nanotube models. <i>Carbohydrate Polymers</i> , 2018, 190, 331-338.	10.2	6
23	Transferability of Sigma Enlarging Bridge Function for Lennard-Jones Diatomic Solute Using Monatomic Solvent Correlation Obtained from Molecular Dynamics Simulation. <i>Chemistry Letters</i> , 2020, 49, 1372-1375.	1.3	6
24	Gibbs Ensemble Monte Carlo Simulation of LJ Fluid in Cylindrical Pore with Energetically Heterogeneous Surface. <i>Molecular Simulation</i> , 2004, 30, 353-359.	2.0	4
25	Extending correlation functions of molecular dynamics simulation by Kovalenko's Hirata and Kobryn's Gusarov's Kovalenko closures for monatomic Lennard-Jones solvent and its application to a calculation of solvation. <i>AIP Advances</i> , 2021, 11, 025026.	1.3	4
26	Brownian Dynamics Simulation of a Spherical Particle in Charged Gel Modeled as Cubic Lattice.. <i>Kagaku Kogaku Ronbunshu</i> , 2001, 27, 42-49.	0.3	1
27	Diffusion of Microparticles in Surfactant Gel.. <i>Kagaku Kogaku Ronbunshu</i> , 2000, 26, 347-353.	0.3	0
28	Accuracy of some useful closure relations in combination with the reference interaction site model theory for fluids of single component diatomic molecules. <i>AIP Advances</i> , 2022, 12, 035248.	1.3	0