# Tatsuhiko Miyata

List of Publications by Year
in descending order

| 28 | 495 | 623734 | 677142 |
|---|---|---|---|
| papers | citations | 14 | 22 |
| | | h-index | g-index |

| 29 | 29 | 29 | 459 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---------|-----|-----------|
| 1 | Accuracy of some useful closure relations in combination with the reference interaction site model theory for fluids of single component diatomic molecules. AIP Advances, 2022, 12, 035248. | 1.3 | 0 |
| 2 | Extending correlation functions of molecular dynamics simulation by Kovalenko–Hirata and Kobryn–Gusarov–Kovalenko closures for monatomic Lennard-Jones solvent and its application to a calculation of solvation. AIP Advances, 2021, 11, 025026. | 1.3 | 4 |
| 3 | Sigma enlarging bridge function for heteronuclear Lennard-Jones diatomic solute solvated in a Lennard-Jones monatomic solvent in terms of the parameter transferability. Chemical Physics Letters, 2020, 755, 137777. | 2.6 | 7 |
| 4 | Transferability of Sigma Enlarging Bridge Function for Lennard-Jones Diatomic Solute Using Monatomic Solvent Correlation Obtained from Molecular Dynamics Simulation. Chemistry Letters, 2020, 49, 1372-1375. | 1.3 | 6 |
| 5 | An assessment of the sigma enlarging bridge function for a Lennard-Jones solution using a solvent-solvent correlation function obtained from molecular dynamics simulation. Journal of Molecular Liquids, 2019, 290, 111167. | 4.9 | 7 |
| 6 | 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. AIP Advances, 2019, 9, . | 1.3 | 9 |
| 7 | Performance of Kobryn-Gusarov-Kovalenko closure from a thermodynamic viewpoint for one-component Lennard-Jones fluids. Chemical Physics Letters, 2018, 700, 88-95. | 2.6 | 14 |
| 8 | Molecular dynamics simulations of theoretical cellulose nanotube models. Carbohydrate Polymers, 2018, 190, 331-338. | 10.2 | 6 |
| 9 | Correction of Kovalenko-Hirata closure in Ornstein-Zernike integral equation theory for Lennard-Jones fluids. Journal of Molecular Liquids, 2017, 245, 2-10. | 4.9 | 17 |
| 10 | A Parameterization of Empirical Sigma Enlarging Bridge Correction of Kovalenko-Hirata Closure in Ornstein-Zernike Theory for Lennard-Jones Fluids. Bulletin of the Chemical Society of Japan, 2017, 90, 1095-1104. | 3.2 | 16 |
| 11 | Accuracy of temperature-derivative of radial distribution function calculated under approximations in Ornstein-Zernike theory for one-component Lennard-Jones fluid. Chemical Physics Letters, 2016, 658, 224-229. | 2.6 | 11 |
| 12 | A pressure consistent bridge correction of Kovalenko-Hirata closure in Ornstein-Zernike theory for Lennard-Jones fluids by apparently adjusting sigma parameter. AIP Advances, 2016, 6, . | 1.3 | 19 |
| 13 | 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. Journal of Molecular Liquids, 2016, 217, 75-82. | 4.9 | 25 |
| 14 | Prediction of cellulose nanotube models through density functional theory calculations. Cellulose, 2014, 21, 87-95. | 4.9 | 7 |
| 15 | Accuracy of solvation free energy calculated by hypernetted chain and Kovalenko–Hirata approximations for two-component system of Lennard-Jones liquid. Chemical Physics Letters, 2014, 604, 122-126. | 2.6 | 23 |
| 16 | Brownian Dynamics Simulation of Self-Diffusion of Ionic Large Solute Molecule in Modeled Polyelectrolyte Gel. Journal of the Physical Society of Japan, 2012, 81, SA010. | 1.6 | 6 |
| 17 | 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. Journal of Chemical Physics, 2011, 134, 044127. | 3.0 | 21 |
| 18 | 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. Journal of Chemical Physics, 2010, 133, 044114. | 3.0 | 36 |

| # | Article | IF | Citations |
|---|---------|----|-----------|
| 19 | Systematic Docking Study of the Carbohydrate Binding Module Protein of Cel7A with the Cellulose Iα Crystal Model. Journal of Physical Chemistry B, 2010, 114, 49-58. | 2.6 | 31 |
| 20 | Molecular Approach To Understand the Tacticity Effects on the Hydrophilicity of Poly(N-isopropylacrylamide): Solubility of Dimer Model Compounds in Water. Journal of Physical Chemistry B, 2010, 114, 13312-13318. | 2.6 | 37 |
| 21 | Combination of molecular dynamics method and 3D–RISM theory for conformational sampling of large flexible molecules in solution. Journal of Computational Chemistry, 2008, 29, 871-882. | 3.3 | 73 |
| 22 | Gibbs Ensemble Monte Carlo Simulation of LJ Fluid in Cylindrical Pore with Energetically Heterogeneous Surface. Molecular Simulation, 2004, 30, 353-359. | 2.0 | 4 |
| 23 | Synthesis of titania-pillared montmorillonite via intercalation of titanium alkoxide dissolved in supercritical carbon dioxide. Journal of Materials Chemistry, 2004, 14, 2763. | 6.7 | 23 |
| 24 | Evaluation of pore size distribution in boundary region of micropore and mesopore using gas adsorption method. Journal of Colloid and Interface Science, 2003, 262, 116-125. | 9.4 | 39 |
| 25 | Brownian Dynamics Simulation Study of Self-Diffusion of a Charged Particle in Swollen Counter-Charged Hydrogel Modeled as Cubic Lattice.. Journal of Chemical Engineering of Japan, 2002, 35, 640-648. | 0.6 | 18 |
| 26 | TiO2–montmorillonite composites via supercritical intercalationElectronic supplementary information (ESI) available: Figs. S1 and S2: powder XRD patterns. See http://www.rsc.org/suppdata/cc/b2/b202589b/. Chemical Communications, 2002, , 1526-1527. | 4.1 | 34 |
| 27 | Brownian Dynamics Simulation of a Spherical Particle in Charged Gel Modeled as Cubic Lattice.. Kagaku Kogaku Ronbunshu, 2001, 27, 42-49. | 0.3 | 1 |
| 28 | Diffusion of Microparticles in Surfactant Gel.. Kagaku Kogaku Ronbunshu, 2000, 26, 347-353. | 0.3 | 0 |