# Nobuyuki Matubayasi

## List of Publications by Citations



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| 233 papers | 5,000 citations | 41 h-index | 58 g-index |
| 251 ext. papers | 5,442 ext. citations | 3.8 avg, IF | 6.18 L-index |

| # | Paper | IF | Citations |
|---|---|---|---|
| 233 | Structural study of supercritical water. I. Nuclear magnetic resonance spectroscopy. *Journal of Chemical Physics*, **1997**, 107, 9133-9140 | 3.9 | 157 |
| 232 | Theory of solutions in the energetic representation. I. Formulation. *Journal of Chemical Physics*, **2000**, 113, 6070-6081 | 3.9 | 133 |
| 231 | Theory of solutions in the energy representation. II. Functional for the chemical potential. *Journal of Chemical Physics*, **2002**, 117, 3605-3616 | 3.9 | 128 |
| 230 | Theory of solutions in the energy representation. III. Treatment of the molecular flexibility. *Journal of Chemical Physics*, **2003**, 119, 9686-9702 | 3.9 | 108 |
| 229 | Thermodynamics of the Hydration Shell. 1. Excess Energy of a Hydrophobic Solute. *The Journal of Physical Chemistry*, **1994**, 98, 10640-10649 | | 107 |
| 228 | NMR Study of Water Structure in Super- and Subcritical Conditions. *Physical Review Letters*, **1997**, 78, 2573-2576 | 7.4 | 103 |
| 227 | Thermodynamics of the Hydration Shell. 2. Excess Volume and Compressibility of a Hydrophobic Solute. *The Journal of Physical Chemistry*, **1996**, 100, 2681-2688 | | 98 |
| 226 | Hydrotropy: monomer-micelle equilibrium and minimum hydrotrope concentration. *Journal of Physical Chemistry B*, **2014**, 118, 10515-24 | 3.4 | 83 |
| 225 | Solvent effect on pathways and mechanisms for D-fructose conversion to 5-hydroxymethyl-2-furaldehyde: in situ 13C NMR study. *Journal of Physical Chemistry A*, **2013**, 117, 2102-13 | 2.8 | 83 |
| 224 | Protein hydration and unfolding--insights from experimental partial specific volumes and unfolded protein models. *Folding & Design*, **1998**, 3, 105-18 | | 81 |
| 223 | A quantum chemical approach to the free energy calculations in condensed systems: the QM/MM method combined with the theory of energy representation. *Journal of Chemical Physics*, **2004**, 121, 3989-99 | 3.9 | 75 |
| 222 | Preferential solvation: dividing surface vs excess numbers. *Journal of Physical Chemistry B*, **2014**, 118, 3922-30 | 3.4 | 74 |
| 221 | The Hofmeister series and protein-salt interactions. *Journal of Chemical Physics*, **2006**, 124, 234905 | 3.9 | 71 |
| 220 | Kinetic and equilibrium study on formic acid decomposition in relation to the water-gas-shift reaction. *Journal of Physical Chemistry A*, **2006**, 110, 11082-90 | 2.8 | 70 |
| 219 | Reversible molecular dynamics for rigid bodies and hybrid Monte Carlo. *Journal of Chemical Physics*, **1999**, 110, 3291-3301 | 3.9 | 70 |
| 218 | Structural study of supercritical water. II. Computer simulations. *Journal of Chemical Physics*, **1999**, 110, 8000-8011 | 3.9 | 70 |
| 217 | Monte Carlo Study of the Effect of Pressure on Hydrophobic Association. *Journal of Physical Chemistry B*, **1997**, 101, 2054-2060 | 3.4 | 69 |

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| 216 | A new high-temperature multinuclear-magnetic-resonance probe and the self-diffusion of light and heavy water in sub- and supercritical conditions. *Journal of Chemical Physics*, **2005**, 123, 164506 | 3.9 | 68 |
| 215 | Structural study of supercritical water. III. Rotational dynamics. *Journal of Chemical Physics*, **2001**, 114, 4107-4115 | 3.9 | 67 |
| 214 | In situ kinetic study on hydrothermal transformation of D-glucose into 5-hydroxymethylfurfural through D-fructose with 13C NMR. *Journal of Physical Chemistry A*, **2011**, 115, 14013-21 | 2.8 | 65 |
| 213 | End-point calculation of solvation free energy of amino-acid analogs by molecular theories of solution. *Chemical Physics Letters*, **2010**, 496, 351-355 | 2.5 | 64 |
| 212 | Free-energy analysis of solubilization in micelle. *Journal of Chemical Physics*, **2006**, 124, 154908 | 3.9 | 61 |
| 211 | Matching-Mismatching of Water Geometry and Hydrophobic Hydration. *Journal of the American Chemical Society*, **1994**, 116, 1450-1456 | 16.4 | 59 |
| 210 | Free-energy analysis of the molecular binding into lipid membrane with the method of energy representation. *Journal of Chemical Physics*, **2008**, 128, 195107 | 3.9 | 57 |
| 209 | Free-energy and structural analysis of ion solvation and contact ion-pair formation of Li(+) with BF4(-) and PF6(-) in water and carbonate solvents. *Journal of Physical Chemistry B*, **2012**, 116, 6476-87 | 3.4 | 54 |
| 208 | Dynamics of Hydrophobic Hydration of Benzene. *The Journal of Physical Chemistry*, **1996**, 100, 1345-1349 | | 54 |
| 207 | Self-diffusion coefficients for water and organic solvents at high temperatures along the coexistence curve. *Journal of Chemical Physics*, **2008**, 129, 214501 | 3.9 | 54 |
| 206 | Gelation of carrageenan: Effects of sugars and polyols. *Food Hydrocolloids*, **2016**, 54, 284-292 | 10.6 | 52 |
| 205 | Ermod: fast and versatile computation software for solvation free energy with approximate theory of solutions. *Journal of Computational Chemistry*, **2014**, 35, 1592-608 | 3.5 | 47 |
| 204 | On the local and nonlocal components of solvation thermodynamics and their relation to solvation shell models. *Journal of Chemical Physics*, **1998**, 109, 4864-4872 | 3.9 | 45 |
| 203 | NMR Spectroscopic Evidence for an Intermediate of Formic Acid in the Water Gas Shift Reaction. *Journal of Physical Chemistry A*, **2004**, 108, 7479-7482 | 2.8 | 45 |
| 202 | Mechanisms and Kinetics of Acetaldehyde Reaction in Supercritical Water: Noncatalytic Disproportionation, Condensation, and Decarbonylation. *Journal of Physical Chemistry A*, **2004**, 108, 11635-11643 | 2.8 | 45 |
| 201 | Gelation: the role of sugars and polyols on gelatin and agarose. *Journal of Physical Chemistry B*, **2014**, 118, 13210-6 | 3.4 | 44 |
| 200 | Controlling the equilibrium of formic acid with hydrogen and carbon dioxide using ionic liquid. *Journal of Physical Chemistry A*, **2010**, 114, 3510-5 | 2.8 | 44 |
| 199 | Preferential hydration of proteins: A Kirkwood-Buff approach. *Chemical Physics Letters*, **2006**, 420, 518-522 | 2.5 | 44 |

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| 198 | The origin of cooperative solubilisation by hydrotropes. *Physical Chemistry Chemical Physics*, **2016**, 18, 25621-25628 | 3.6 | 42 |
| 197 | Communication: Free-energy analysis of hydration effect on protein with explicit solvent: equilibrium fluctuation of cytochrome c. *Journal of Chemical Physics*, **2011**, 134, 041105 | 3.9 | 42 |
| 196 | Hydrothermal reactions of formaldehyde and formic acid: free-energy analysis of equilibrium. *Journal of Chemical Physics*, **2005**, 122, 074509 | 3.9 | 42 |
| 195 | Hydrothermal carbon-carbon bond formation and disproportionations of C1 aldehydes: formaldehyde and formic acid. *Journal of Physical Chemistry A*, **2005**, 109, 6610-9 | 2.8 | 41 |
| 194 | Structure and dynamics of water: from ambient to supercritical. *Journal of Molecular Liquids*, **2001**, 90, 75-83 | 6 | 41 |
| 193 | Evaluation of protein-protein docking model structures using all-atom molecular dynamics simulations combined with the solution theory in the energy representation. *Journal of Chemical Physics*, **2012**, 137, 215105 | 3.9 | 39 |
| 192 | A novel quantum mechanical/molecular mechanical approach to the free energy calculation for isomerization of glycine in aqueous solution. *Journal of Chemical Physics*, **2005**, 123, 124504 | 3.9 | 38 |
| 191 | Energetic origin of proton affinity to the air/water interface. *Journal of Physical Chemistry B*, **2011**, 115, 4745-51 | 3.4 | 37 |
| 190 | Self-Consistent Determination of Atomic Charges of Ionic Liquid through a Combination of Molecular Dynamics Simulation and Density Functional Theory. *Journal of Chemical Theory and Computation*, **2016**, 12, 804-11 | 6.4 | 36 |
| 189 | Slowdown of H/D exchange reaction rate and water dynamics in ionic liquids: deactivation of solitary water solvated by small anions in 1-butyl-3-methyl-imidazolium chloride. *Journal of Physical Chemistry A*, **2007**, 111, 541-3 | 2.8 | 36 |
| 188 | Pair-correlation entropy of hydrophobic hydration: decomposition into translational and orientational contributions and analysis of solute-size effects. *Journal of Chemical Physics*, **2006**, 124, 024512 | 3.9 | 36 |
| 187 | Super- and subcritical hydration of nonpolar solutes. I. Thermodynamics of hydration. *Journal of Chemical Physics*, **2000**, 112, 8089-8109 | 3.9 | 36 |
| 186 | Gastrophysics: Statistical thermodynamics of biomolecular denaturation and gelation from the Kirkwood-Buff theory towards the understanding of tofu. *Food Hydrocolloids*, **2017**, 62, 128-139 | 10.6 | 35 |
| 185 | Rotational dynamics of water and benzene controlled by anion field in ionic liquids: 1-butyl-3-methylimidazolium chloride and hexafluorophosphate. *Journal of Chemical Physics*, **2007**, 127, 104506 | 3.9 | 34 |
| 184 | Hot Water Induces an Acid-Catalyzed Reaction in Its Undissociated Form. *Bulletin of the Chemical Society of Japan*, **2004**, 77, 691-697 | 5.1 | 34 |
| 183 | Self-diffusion of supercritical water in extremely low-density region. *Journal of Chemical Physics*, **2006**, 125, 074307 | 3.9 | 33 |
| 182 | Effect of Concentration, Acid, Temperature, and Metal on Competitive Reaction Pathways for Decarbonylation and Decarboxylation of Formic Acid in Hot Water. *Chemistry Letters*, **2004**, 33, 572-573 | 1.7 | 33 |
| 181 | Which carbon oxide is more soluble? Ab initio study on carbon monoxide and dioxide in aqueous solution. *Chemical Physics Letters*, **2000**, 323, 257-262 | 2.5 | 33 |

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| 180 | Unifying hydrotropy under Gibbs phase rule. *Physical Chemistry Chemical Physics*, **2017**, 19, 23597-23605 | 3.6 | 31 |
| 179 | Computation of the free energy change associated with one-electron reduction of coenzyme immersed in water: a novel approach within the framework of the quantum mechanical/molecular mechanical method combined with the theory of energy representation. *Journal of Chemical Physics*, **2008**, 129, 205103 | 3.9 | 31 |
| 178 | Interaction-component analysis of the urea effect on amino acid analogs. *Physical Chemistry Chemical Physics*, **2013**, 15, 4377-91 | 3.6 | 30 |
| 177 | Noncatalytic Cannizzaro-type Reaction of Acetaldehyde in Supercritical Water. *Chemistry Letters*, **2003**, 32, 310-311 | 1.7 | 28 |
| 176 | Hydration property of globular proteins: An analysis of solvation free energy by energy representation method. *Chemical Physics Letters*, **2010**, 497, 218-222 | 2.5 | 27 |
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| 174 | Interaction-component analysis of the hydration and urea effects on cytochrome c. *Journal of Chemical Physics*, **2016**, 144, 085102 | 3.9 | 26 |
| 173 | Free-energy analysis of water affinity in polymer studied by atomistic molecular simulation combined with the theory of solutions in the energy representation. *Journal of Chemical Physics*, **2012**, 137, 234903 | 3.9 | 25 |
| 172 | A unified perspective on preferential solvation and adsorption based on inhomogeneous solvation theory. *Physica A: Statistical Mechanics and Its Applications*, **2018**, 492, 1988-1996 | 3.3 | 25 |
| 171 | Origin of non-linearity in phase solubility: solubilisation by cyclodextrin beyond stoichiometric complexation. *Physical Chemistry Chemical Physics*, **2016**, 18, 15205-17 | 3.6 | 24 |
| 170 | NMR Study on the Reorientational Relaxation in Supercritical Alcohols. *Journal of Physical Chemistry A*, **2004**, 108, 1319-1324 | 2.8 | 23 |
| 169 | Enthalpy and Entropy Decomposition of Free-Energy Changes for Side-Chain Conformations of Aspartic Acid and Asparagine in Acidic, Neutral, and Basic Aqueous Solutions. *Journal of Physical Chemistry B*, **2002**, 106, 12336-12343 | 3.4 | 23 |
| 168 | Kinetic study on disproportionations of C1 aldehydes in supercritical water: methanol from formaldehyde and formic acid. *Journal of Physical Chemistry A*, **2007**, 111, 2697-705 | 2.8 | 22 |
| 167 | Solvation shell dynamics studied by molecular dynamics simulation in relation to the translational and rotational dynamics of supercritical water and benzene. *Journal of Chemical Physics*, **2007**, 127, 174509 | 3.9 | 22 |
| 166 | Chloride Ion Hydration and Diffusion in Supercritical Water Using a Polarizable Water Model. *Journal of Physical Chemistry B*, **2002**, 106, 3979-3986 | 3.4 | 22 |
| 165 | Investigation of the dominant hydration structures among the ionic species in aqueous solution: novel quantum mechanics/molecular mechanics simulations combined with the theory of energy representation. *Journal of Chemical Physics*, **2008**, 128, 064507 | 3.9 | 21 |
| 164 | Free-energy analysis of protein solvation with all-atom molecular dynamics simulation combined with a theory of solutions. *Current Opinion in Structural Biology*, **2017**, 43, 45-54 | 8.1 | 20 |
| 163 | Structural characteristics of yeast F1-ATPase before and after 16-degree rotation of the □subunit: theoretical analysis focused on the water-entropy effect. *Journal of Chemical Physics*, **2012**, 137, 035102 | 3.9 | 20 |

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| 162 | Limited slowdown of endocrine-disruptor diffusion in confined fluid lipid membranes. *Physical Review Letters*, **2004**, 93, 248101 | 7.4 | 20 |
| 161 | Noncatalytic Disproportionation and Decarbonylation Reactions of Benzaldehyde in Supercritical Water. *Chemistry Letters*, **2004**, 33, 622-623 | 1.7 | 20 |
| 160 | Energetics of nonpolar and polar compounds in cationic, anionic, and nonionic micelles studied by all-atom molecular dynamics simulation combined with a theory of solutions. *Physical Chemistry Chemical Physics*, **2016**, 18, 13223-31 | 3.6 | 20 |
| 159 | Spatial-Decomposition Analysis of Energetics of Ionic Hydration. *Journal of Physical Chemistry B*, **2016**, 120, 1813-21 | 3.4 | 19 |
| 158 | Molecular dynamics study of fast dielectric relaxation of water around a molecular-sized ion. *Journal of Chemical Physics*, **2012**, 137, 224502 | 3.9 | 19 |
| 157 | Energy-Representation Theory of Solutions: Its Formulation and Application to Soft, Molecular Aggregates. *Bulletin of the Chemical Society of Japan*, **2019**, 92, 1910-1927 | 5.1 | 19 |
| 156 | The Role of Interfacial Water in Protein-Ligand Binding: Insights from the Indirect Solvent Mediated Potential of Mean Force. *Journal of Chemical Theory and Computation*, **2018**, 14, 512-526 | 6.4 | 18 |
| 155 | Correlation analysis for heat denaturation of Trp-cage miniprotein with explicit solvent. *Protein Science*, **2016**, 25, 56-66 | 6.3 | 18 |
| 154 | The mechanism of salt effects on starch gelatinization from a statistical thermodynamic perspective. *Food Hydrocolloids*, **2019**, 87, 593-601 | 10.6 | 18 |
| 153 | Scaled Polynomial Expression for Self-Diffusion Coefficients for Water, Benzene, and Cyclohexane over a Wide Range of Temperatures and Densities. *Journal of Chemical & Engineering Data*, **2010**, 55, 2815-2823 | 2.8 | 18 |
| 152 | Communication: exploring the reorientation of benzene in an ionic liquid via molecular dynamics: effect of temperature and solvent effective charge on the slow dynamics. *Journal of Chemical Physics*, **2011**, 134, 191101 | 3.9 | 18 |
| 151 | Nuclear magnetic resonance study on rotational dynamics of water and benzene in a series of ionic liquids: anion and cation effects. *Journal of Chemical Physics*, **2012**, 137, 194503 | 3.9 | 18 |
| 150 | Mechanisms and kinetics of noncatalytic ether reaction in supercritical water. 2. Proton-transferred fragmentation of dimethyl ether to formaldehyde in competition with hydrolysis. *Journal of Physical Chemistry A*, **2005**, 109, 3558-64 | 2.8 | 18 |
| 149 | Molecular dynamics simulations of yeast F1-ATPase before and after 16° rotation of the γ subunit. *Journal of Physical Chemistry B*, **2013**, 117, 3298-307 | 3.4 | 17 |
| 148 | A theoretical study of the two binding modes between lysozyme and tri-NAG with an explicit solvent model based on the fragment molecular orbital method. *Physical Chemistry Chemical Physics*, **2013**, 15, 3646-54 | 3.6 | 17 |
| 147 | Insights into the origins of configurational stability of axially chiral biaryl amines with an intramolecular N-H-N hydrogen bond. *Journal of Organic Chemistry*, **2010**, 75, 5031-6 | 4.2 | 17 |
| 146 | Acid-Catalyzed Hydrothermal Formation of Carbon−Carbon Bond in Glycolic Acid from a Series of Formaldehyde Producers. *Chemistry Letters*, **2004**, 33, 624-625 | 1.7 | 17 |
| 145 | Jump in the Rotational Mobility of Benzene Induced by the Clathrate Hydrate Formation. *The Journal of Physical Chemistry*, **1995**, 99, 1377-1379 | | 17 |

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| 144 | Hydrotropy and scattering: pre-ouzo as an extended near-spinodal region. *Physical Chemistry Chemical Physics*, **2017**, 19, 26734-26742 | 3.6 | 16 |
| 143 | Spatial-decomposition analysis of electrical conductivity in concentrated electrolyte solution. *Journal of Chemical Physics*, **2014**, 141, 044126 | 3.9 | 16 |
| 142 | Simple and exact approach to the electronic polarization effect on the solvation free energy: formulation for quantum-mechanical/molecular-mechanical system and its applications to aqueous solutions. *Journal of Chemical Physics*, **2012**, 136, 214503 | 3.9 | 16 |
| 141 | Association and Dissociation of Nonpolar Solutes in Super- and Subcritical Water. *Journal of Physical Chemistry B*, **2000**, 104, 10352-10358 | 3.4 | 16 |
| 140 | Free-Energy Analysis of Peptide Binding in Lipid Membrane Using All-Atom Molecular Dynamics Simulation Combined with Theory of Solutions. *Journal of Physical Chemistry B*, **2018**, 122, 3219-3229 | 3.4 | 15 |
| 139 | Effective charges of ionic liquid determined self-consistently through combination of molecular dynamics simulation and density-functional theory. *Journal of Computational Chemistry*, **2017**, 38, 2559-2569 | 3.5 | 15 |
| 138 | Computation of the reduction free energy of coenzyme in aqueous solution by the QM/MM-ER method. *Chemical Physics Letters*, **2008**, 456, 176-180 | 2.5 | 15 |
| 137 | Noncatalytic kinetic study on site-selective H/D exchange reaction of phenol in sub- and supercritical water. *Journal of Chemical Physics*, **2004**, 121, 960-9 | 3.9 | 15 |
| 136 | Tumbling and spinning diffusions of acetonitrile in water and organic solvents. *Journal of Chemical Physics*, **2000**, 112, 1462-1473 | 3.9 | 15 |
| 135 | Boson peak, elasticity, and glass transition temperature in polymer glasses: Effects of the rigidity of chain bending. *Scientific Reports*, **2019**, 9, 19514 | 4.9 | 15 |
| 134 | Water activity in liquid food systems: A molecular scale interpretation. *Food Chemistry*, **2017**, 237, 1133-1138 | 5.9 | 14 |
| 133 | Binding free energy analysis of protein-protein docking model structures by evERdock. *Journal of Chemical Physics*, **2018**, 148, 105101 | 3.9 | 14 |
| 132 | Cholesterol location and orientation in aqueous suspension of large unilamellar vesicles of phospholipid revealed by intermolecular nuclear overhauser effect. *Journal of Physical Chemistry B*, **2008**, 112, 2622-8 | 3.4 | 14 |
| 131 | Mechanisms and kinetics of noncatalytic ether reaction in supercritical water. 1. Proton-transferred fragmentation of diethyl ether to acetaldehyde in competition with hydrolysis. *Journal of Physical Chemistry A*, **2005**, 109, 3550-7 | 2.8 | 14 |
| 130 | Dynamic and 2D NMR studies on hydrogen-bonding aggregates of cholesterol in low-polarity organic solvents. *Journal of Physical Chemistry B*, **2006**, 110, 15205-11 | 3.4 | 14 |
| 129 | Computing conformational free energy differences in explicit solvent: An efficient thermodynamic cycle using an auxiliary potential and a free energy functional constructed from the end points. *Journal of Computational Chemistry*, **2017**, 38, 1198-1208 | 3.5 | 13 |
| 128 | NMR-NOE and MD simulation study on phospholipid membranes: dependence on membrane diameter and multiple time scale dynamics. *Journal of Physical Chemistry B*, **2011**, 115, 9106-15 | 3.4 | 13 |
| 127 | Distribution-function approach to free energy computation. *Journal of Chemical Physics*, **2011**, 135, 114108 | 3.9 | 13 |

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| 126 | Rotational dynamics of benzene and water in an ionic liquid explored via molecular dynamics simulations and NMR T1 measurements. *Journal of Chemical Physics*, **2012**, 136, 074508 | 3.9 | 13 |
| 125 | Water as an in situ NMR indicator for impurity acids in ionic liquids. *Analytical Chemistry*, **2009**, 81, 400-7 | 7.8 | 13 |
| 124 | 14N NMR Spectra Sensitively Reflect Surface Curvature and Segmental Motion of Hydrophilic Headgroups in Lipid Bilayers and Micelles. *Chemistry Letters*, **1997**, 26, 1061-1062 | 1.7 | 13 |
| 123 | High-Sensitivity Raman Spectroscopy of Supercritical Water and Methanol over a Wide Range of Density. *Bulletin of the Chemical Society of Japan*, **2007**, 80, 1764-1769 | 5.1 | 13 |
| 122 | Carbon□Carbon Bond Formation in Glycolic Acid Generated Spontaneously from Dichloromethane in Hot Water. *Chemistry Letters*, **2004**, 33, 302-303 | 1.7 | 13 |
| 121 | Real-time In-cell19F NMR Study on Uptake of Fluorescent and Nonfluorescent19F-Octaarginines into Human Jurkat Cells. *Chemistry Letters*, **2005**, 34, 1064-1065 | 1.7 | 13 |
| 120 | Drastic Compensation of Electronic and Solvation Effects on ATP Hydrolysis Revealed through Large-Scale QM/MM Simulations Combined with a Theory of Solutions. *Journal of Physical Chemistry B*, **2017**, 121, 2279-2287 | 3.4 | 12 |
| 119 | Relationship between Solvation Thermodynamics from IST and DFT Perspectives. *Journal of Physical Chemistry B*, **2017**, 121, 3825-3841 | 3.4 | 12 |
| 118 | Statistical thermodynamic foundation for mesoscale aggregation in ternary mixtures. *Physical Chemistry Chemical Physics*, **2018**, 20, 13777-13784 | 3.6 | 12 |
| 117 | Structure and permeability of ionomers studied by atomistic molecular simulation combined with the theory of solutions in the energy representation. *Journal of Chemical Physics*, **2018**, 148, 214903 | 3.9 | 12 |
| 116 | Finite-size effect on the charging free energy of protein in explicit solvent. *Journal of Chemical Theory and Computation*, **2015**, 11, 215-23 | 6.4 | 12 |
| 115 | Energetic contributions from the cation and anion to the stability of carbon dioxide dissolved in imidazolium-based ionic liquids. *Journal of Physical Chemistry B*, **2015**, 119, 1579-87 | 3.4 | 12 |
| 114 | Self-diffusion coefficients for water and organic solvents in extremely low-density supercritical states. *Journal of Molecular Liquids*, **2009**, 147, 96-101 | 6 | 12 |
| 113 | NMR Study of Water Structure in Super- and Subcritical Conditions [Phys. Rev. Lett. 78, 2573 (1997)]. *Physical Review Letters*, **1997**, 78, 4309-4309 | 7.4 | 12 |
| 112 | Comparative study on the properties of hydration water of Na- and K-halide ions by Raman OH/OD-stretching spectroscopy and dielectric relaxation data. *Journal of Physical Chemistry A*, **2014**, 118, 2922-30 | 2.8 | 11 |
| 111 | Spatial-decomposition analysis of electrical conductivity in ionic liquid. *Journal of Chemical Physics*, **2014**, 141, 244507 | 3.9 | 11 |
| 110 | Density effect on infrared spectrum for supercritical water in the low- and medium-density region studied by molecular dynamics simulation. *Journal of Chemical Physics*, **2012**, 137, 194506 | 3.9 | 11 |
| 109 | NMR study on the binding of neuropeptide achatin-I to phospholipid bilayer: the equilibrium, location, and peptide conformation. *Biophysical Journal*, **2004**, 87, 375-85 | 2.9 | 11 |

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| 108 | Nuclear magnetic resonance and molecular dynamics simulation study on the reorientational relaxation of solutes in supercritical methanol. *Journal of Molecular Liquids*, **2005**, 119, 119-123 | 6 | 11 |
| 107 | Refining evERdock: Improved selection of good protein-protein complex models achieved by MD optimization and use of multiple conformations. *Journal of Chemical Physics*, **2018**, 149, 195101 | 3.9 | 11 |
| 106 | Osmolyte depletion viewed in terms of the dividing membrane and its work of expansion against osmotic pressure. *Biophysical Chemistry*, **2017**, 231, 111-115 | 3.5 | 10 |
| 105 | MD simulation analysis of resin filling into nano-sized pore formed on metal surface. *Applied Surface Science*, **2018**, 427, 1084-1091 | 6.7 | 10 |
| 104 | Noncatalytic hydrothermal elimination of the terminal D-glucose unit from malto- and cello-oligosaccharides through transformation to D-fructose. *Journal of Physical Chemistry A*, **2012**, 116, 10039-49 | 2.8 | 10 |
| 103 | Hydration structure around CO2 captured in aqueous amine solutions observed by high energy X-ray scattering. *International Journal of Greenhouse Gas Control*, **2011**, 5, 1533-1539 | 4.2 | 10 |
| 102 | Partial pair correlation functions of low-density supercritical water determined by neutron diffraction with the H/D isotopic substitution method. *Journal of Physical Chemistry B*, **2008**, 112, 4687-93 | 3.4 | 10 |
| 101 | Diffusion dynamics of supercooled water modeled with the cage-jump motion and hydrogen-bond rearrangement. *Journal of Chemical Physics*, **2019**, 150, 204502 | 3.9 | 9 |
| 100 | Spatially-Decomposed Free Energy of Solvation Based on the Endpoint Density-Functional Method. *Journal of Chemical Theory and Computation*, **2019**, 15, 2896-2912 | 6.4 | 9 |
| 99 | Resin filling into nano-sized pore on metal surface analyzed by all-atom molecular dynamics simulation over a variety of resin and pore sizes. *Polymer*, **2018**, 150, 360-370 | 3.9 | 9 |
| 98 | Anion-dependence of fast relaxation component in Na-, K-halide solutions at low concentrations measured by high-resolution microwave dielectric spectroscopy. *Journal of Physical Chemistry A*, **2013**, 117, 4851-62 | 2.8 | 9 |
| 97 | Molecular insights on confined water in the nanochannels of self-assembled ionic liquid crystal. *Science Advances*, **2021**, 7, | 14.3 | 9 |
| 96 | Free-energy analysis of the hydration and cosolvent effects on the β-sheet aggregation through all-atom molecular dynamics simulation. *Journal of Chemical Physics*, **2019**, 150, 145101 | 3.9 | 8 |
| 95 | Probabilistic analysis for identifying the driving force of protein folding. *Journal of Chemical Physics*, **2018**, 148, 125101 | 3.9 | 8 |
| 94 | Free-energy analysis of lysozyme–triNAG binding modes with all-atom molecular dynamics simulation combined with the solution theory in the energy representation. *Chemical Physics Letters*, **2013**, 559, 94-98 | 2.5 | 8 |
| 93 | Interaction-component analysis of the effects of urea and its alkylated derivatives on the structure of T4-lysozyme. *Journal of Chemical Physics*, **2017**, 146, 225103 | 3.9 | 8 |
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| 91 | Free-energy analysis of the electron-density fluctuation in the quantum-mechanical/molecular-mechanical simulation combined with the theory of energy representation. *Journal of Chemical Physics*, **2012**, 136, 044505 | 3.9 | 8 |

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| 90 | Hydrothermal C-C bond formation and disproportionation of acetaldehyde with formic acid. *Journal of Physical Chemistry A*, **2008**, 112, 6950-9 | 2.8 | 8 |
| 89 | Pressure Effect on Hydrophobic Hydration: Rotational Dynamics of Benzene. *Journal of Physical Chemistry A*, **1999**, 103, 6685-6690 | 2.8 | 8 |
| 88 | Self-Consistent Scheme Combining MD and Order- DFT Methods: An Improved Set of Nonpolarizable Force Fields for Ionic Liquids. *Journal of Chemical Theory and Computation*, **2020**, 16, 651-665 | 6.4 | 8 |
| 87 | Learning reaction coordinates via cross-entropy minimization: Application to alanine dipeptide. *Journal of Chemical Physics*, **2020**, 153, 054115 | 3.9 | 8 |
| 86 | Structure and Dynamics of the Hydration Shell: Spatially Decomposed Time Correlation Approach. *Journal of Chemical Theory and Computation*, **2019**, 15, 803-812 | 6.4 | 8 |
| 85 | The Excess Chemical Potential of Water at the Interface with a Protein from End Point Simulations. *Journal of Physical Chemistry B*, **2018**, 122, 4700-4707 | 3.4 | 7 |
| 84 | Quantifying non-specific interactions between flavour and food biomolecules. *Food and Function*, **2017**, 8, 2999-3009 | 6.1 | 7 |
| 83 | Effect of heavy hydrogen isotopes on the vibrational line shape for supercritical water through rotational couplings. *Journal of Chemical Physics*, **2013**, 138, 134508 | 3.9 | 7 |
| 82 | The effect of pressure on halothane binding to hydrated DMPC bilayers. *Molecular Physics*, **2012**, 110, 1461-1467 | 1.7 | 7 |
| 81 | Free-energy change of inserting halothane into different depths of a hydrated DMPC bilayer. *Chemical Physics Letters*, **2008**, 462, 112-115 | 2.5 | 7 |
| 80 | An approach to the solvation free energy in terms of the distribution functions of the solute–solvent interaction energy. *Journal of Molecular Liquids*, **2005**, 119, 23-29 | 6 | 7 |
| 79 | Solubilization power of surfactant-free microemulsions. *Physical Chemistry Chemical Physics*, **2020**, 22, 22185-22189 | 3.6 | 7 |
| 78 | Transport Properties of Ionic Liquid and Sodium Salt Mixtures for Sodium-Ion Battery Electrolytes from Molecular Dynamics Simulation with a Self-Consistent Atomic Charge Determination. *Journal of Physical Chemistry B*, **2020**, 124, 7291-7305 | 3.4 | 7 |
| 77 | Fluctuation adsorption theory: quantifying adsorbate-adsorbate interaction and interfacial phase transition from an isotherm. *Physical Chemistry Chemical Physics*, **2020**, 22, 28304-28316 | 3.6 | 7 |
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| 73 | Side-chain conformational thermodynamics of aspartic acid residue in the peptides and achatin-I in aqueous solution. *Biophysical Journal*, **2004**, 86, 1124-37 | 2.9 | 6 |

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