Nobuyuki Matubayasi

List of Publications by Year in Descending Order

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	Simulating the nematic-isotropic phase transition of liquid crystal model via generalized replica-exchange method.. *Journal of Chemical Physics*, **2022**, 156, 014901	3.9	1
232	Ensemble transformation in the fluctuation theory. *Physica A: Statistical Mechanics and Its Applications*, **2022**, 585, 126430	3.3	0
231	Explaining reaction coordinates of alanine dipeptide isomerization obtained from deep neural networks using Explainable Artificial Intelligence (XAI).. *Journal of Chemical Physics*, **2022**, 156, 154108	3.9	1
230	Molecular Structure and Vibrational Spectra of Water Molecules Sorbed in Poly(2-methoxyethylacrylate) Revealed by Molecular Dynamics Simulation. *Journal of Physical Chemistry B*, **2021**, 125, 12095-12103	3.4	1
229	Atomistic description of molecular binding processes based on returning probability theory. *Journal of Chemical Physics*, **2021**, 155, 204503	3.9	0
228	Spatial-Decomposition Analysis of Electrical Conductivity in Mixtures of Ionic Liquid and Sodium Salt for Sodium-Ion Battery Electrolytes. *Journal of Physical Chemistry B*, **2021**, 125, 3374-3385	3.4	2
227	Implicit function theorem and Jacobians in solvation and adsorption. *Physica A: Statistical Mechanics and Its Applications*, **2021**, 570, 125801	3.3	5
226	Understanding the scaling of boson peak through insensitivity of elastic heterogeneity to bending rigidity in polymer glasses. *Journal of Physics Condensed Matter*, **2021**, 33,	1.8	2
225	Transition pathway of hydrogen bond switching in supercooled water analyzed by the Markov state model. *Journal of Chemical Physics*, **2021**, 154, 234501	3.9	0
224	Sorption: A Statistical Thermodynamic Fluctuation Theory. *Langmuir*, **2021**, 37, 7380-7391	4	6
223	Phase stability condition and liquid–liquid phase separation under mesoscale confinement. *Physica A: Statistical Mechanics and Its Applications*, **2021**, 563, 125385	3.3	6
222	Construction of isostructural hydrogen-bonded organic frameworks: limitations and possibilities of pore expansion. *Chemical Science*, **2021**, 12, 9607-9618	9.4	6
221	Solvation energetics of proteins and their aggregates analyzed by all-atom molecular dynamics simulations and the energy-representation theory of solvation. *Chemical Communications*, **2021**, 57, 9968-9978	5.8	0
220	Cooperativity in micellar solubilization. *Physical Chemistry Chemical Physics*, **2021**, 23, 8705-8716	3.6	3
219	Molecular insights on confined water in the nanochannels of self-assembled ionic liquid crystal. *Science Advances*, **2021**, 7,	14.3	9
218	Cooperative Sorption on Porous Materials. *Langmuir*, **2021**, 37, 10279-10290	4	5
217	Adsorbate-adsorbate interactions on microporous materials. *Microporous and Mesoporous Materials* , **2021**, 323, 111254	5.3	5

216	Water Dissolved in a Variety of Polymers Studied by Molecular Dynamics Simulation and a Theory of Solutions. *Journal of Physical Chemistry B*, **2021**, 125, 9357-9371	3.4	4
215	Temperature Dependence of Sorption. *Langmuir*, **2021**, 37, 11008-11017	4	0
214	Crystallization of Polyethylene Brushes and Its Effect on Interactions with Water. *Macromolecules*, **2021**, 54, 8303-8313	5.5	
213	Breakdown of the Stokes-Einstein relation in supercooled liquids: A cage-jump perspective. *Journal of Chemical Physics*, **2021**, 155, 114503	3.9	0
212	Effects of chain length on Rouse modes and non-Gaussianity in linear and ring polymer melts. *Journal of Chemical Physics*, **2021**, 155, 124901	3.9	0
211	Solvation Thermodynamics from the Perspective of Endpoints DFT. *Journal of Physical Chemistry B*, **2020**, 124, 11771-11782	3.4	0
210	Cavity Particle in Aqueous Solution with a Hydrophobic Solute: Structure, Energetics, and Functionals. *Journal of Physical Chemistry B*, **2020**, 124, 5220-5237	3.4	1
209	Chain-Increment Method for Free-Energy Computation of a Polymer with All-Atom Molecular Simulations. *Macromolecules*, **2020**, 53, 775-788	5.5	3
208	Thermodynamic stability condition can judge whether a nanoparticle dispersion can be considered a solution in a single phase. *Journal of Colloid and Interface Science*, **2020**, 575, 472-479	9.3	5
207	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
206	Intensive nature of fluctuations: Reconceptualizing Kirkwood-Buff theory via elementary algebra. *Journal of Molecular Liquids*, **2020**, 318, 114225	6	6
205	Solubilization power of surfactant-free microemulsions. *Physical Chemistry Chemical Physics*, **2020**, 22, 22185-22189	3.6	7
204	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
203	Learning reaction coordinates via cross-entropy minimization: Application to alanine dipeptide. *Journal of Chemical Physics*, **2020**, 153, 054115	3.9	8
202	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
201	Consistency of geometrical definitions of hydrogen bonds based on the two-dimensional potential of mean force with respect to the time correlation in liquid water over a wide range of temperatures. *Journal of Molecular Liquids*, **2019**, 294, 111603	6	2
200	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
199	Bridging the gap between molecular dynamics and hydrodynamics in nanoscale Brownian motions. *Soft Matter*, **2019**, 15, 4380-4390	3.6	4

198	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
197	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
196	The mechanism of salt effects on starch gelatinization from a statistical thermodynamic perspective. *Food Hydrocolloids*, **2019**, 87, 593-601	10.6	18
195	Local viscoelasticity at resin-metal interface analyzed with spatial-decomposition formula for relaxation modulus. *Journal of Chemical Physics*, **2019**, 151, 114904	3.9	1
194	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
193	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
192	Energetics of cosolvent effect on peptide aggregation. *Biophysics and Physicobiology*, **2019**, 16, 185-195	1.4	1
191	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
190	A Molecular Thermodynamics Approach to Capture Non-specific Flavour–Macromolecule Interactions **2019**, 522-527		
189	Statistical thermodynamics of regular solutions and solubility parameters. *Journal of Molecular Liquids*, **2019**, 273, 626-633	6	1
188	Spatial-decomposition analysis of viscosity with application to Lennard-Jones fluid. *Journal of Chemical Physics*, **2018**, 148, 094501	3.9	5
187	Probabilistic analysis for identifying the driving force of protein folding. *Journal of Chemical Physics*, **2018**, 148, 125101	3.9	8
186	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
185	Ion hydration: linking self-diffusion and reorientational motion to water structure. *Physical Chemistry Chemical Physics*, **2018**, 20, 5909-5917	3.6	6
184	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
183	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
182	Binding free energy analysis of protein-protein docking model structures by evERdock. *Journal of Chemical Physics*, **2018**, 148, 105101	3.9	14
181	MD simulation analysis of resin filling into nano-sized pore formed on metal surface. *Applied Surface Science*, **2018**, 427, 1084-1091	6.7	10

180	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
179	How do hydrogen bonds break in supercooled water?: Detecting pathways not going through saddle point of two-dimensional potential of mean force. *Journal of Chemical Physics*, **2018**, 148, 244501	3.9	5
178	Free-energy analysis of physisorption on solid-liquid interface with the solution theory in the energy representation. *Journal of Chemical Physics*, **2018**, 149, 014504	3.9	4
177	Statistical thermodynamic foundation for mesoscale aggregation in ternary mixtures. *Physical Chemistry Chemical Physics*, **2018**, 20, 13777-13784	3.6	12
176	Novel Intermolecular Surface Force Unveils the Driving Force of the Actomyosin System **2018**, 257-274		1
175	Spatial Distribution of Ionic Hydration Energy and Hyper-Mobile Water **2018**, 33-52		1
174	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
173	Spatial-Decomposition Analysis of Electrical Conductivity. *Chemical Record*, **2018**, 19, 723	6.6	5
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	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
170	All-Atom Analysis of Free Energy of Protein Solvation Through Molecular Simulation and Solution Theory **2018**, 141-155		
169	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
168	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
167	Relationship between Solvation Thermodynamics from IST and DFT Perspectives. *Journal of Physical Chemistry B*, **2017**, 121, 3825-3841	3.4	12
166	Energetic Analysis of Adsorption and Absorption of Small Molecule to Nanodroplet of Water. *Journal of Physical Chemistry B*, **2017**, 121, 5995-6001	3.4	4
165	Unifying hydrotropy under Gibbs phase rule. *Physical Chemistry Chemical Physics*, **2017**, 19, 23597-23605	3.6	31
164	Water activity in liquid food systems: A molecular scale interpretation. *Food Chemistry*, **2017**, 237, 1133-1138		14
163	Protein-Protein Complex Structure Prediction using the Solution Theory in the Energy Representation. *Biophysical Journal*, **2017**, 112, 53a-54a	2.9	

162	Pseudomonas aeruginosa cytochrome c denaturation by five systematic urea derivatives that differ in the alkyl chain length. *Bioscience, Biotechnology and Biochemistry*, **2017**, 81, 1274-1278	2.1	4
161	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
160	Hydrotropy and scattering: pre-ouzo as an extended near-spinodal region. *Physical Chemistry Chemical Physics*, **2017**, 19, 26734-26742	3.6	16
159	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
158	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
157	Quantifying non-specific interactions between flavour and food biomolecules. *Food and Function*, **2017**, 8, 2999-3009	6.1	7
156	Physical driving force of actomyosin motility based on the hydration effect. *Cytoskeleton*, **2017**, 74, 512-527	2.4	8
155	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
154	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
153	Energy Representation Approach **2017**,		
152	The origin of cooperative solubilisation by hydrotropes. *Physical Chemistry Chemical Physics*, **2016**, 18, 25621-25628	3.6	42
151	Effect of Rotation on Vibrational Spectrum of Supercritical Water: Analysis of Dependencies on Density and Hydrogen Isotopes. *Review of High Pressure Science and Technology/Koatsuryoku No Kagaku To Gijutsu*, **2016**, 26, 323-332	0	1
150	Morphology study of DMPC/DHPC mixtures by solution-state 1H, 31P NMR, and NOE measurements. *Journal of Molecular Liquids*, **2016**, 217, 62-69	6	5
149	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
148	Spatial-Decomposition Analysis of Energetics of Ionic Hydration. *Journal of Physical Chemistry B*, **2016**, 120, 1813-21	3.4	19
147	Correlation analysis for heat denaturation of Trp-cage miniprotein with explicit solvent. *Protein Science*, **2016**, 25, 56-66	6.3	18
146	Gelation of carrageenan: Effects of sugars and polyols. *Food Hydrocolloids*, **2016**, 54, 284-292	10.6	52
145	Interaction-component analysis of the hydration and urea effects on cytochrome c. *Journal of Chemical Physics*, **2016**, 144, 085102	3.9	26

144	Origin of non-linearity in phase solubility: solubilisation by cyclodextrin beyond stoichiometric complexation. *Physical Chemistry Chemical Physics*, **2016**, 18, 15205-17	3.6	24
143	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
142	An accurate and efficient computation method of the hydration free energy of a large, complex molecule. *Journal of Chemical Physics*, **2015**, 142, 175101	3.9	6
141	Free-energy Analysis of Binding Functions of Soft Molecular Aggregates on the Basis of the Extended Concept of Solvation. *Bunseki Kagaku*, **2015**, 64, 185-188	0.2	
140	Effect of diffuseness of micelle boundary on the solute distribution upon solubilization. *Chemical Physics Letters*, **2015**, 624, 19-23	2.5	4
139	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
138	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
137	Development of a Massively Parallel QM/MM Approach Combined with a Theory of Solutions. *Challenges and Advances in Computational Chemistry and Physics*, **2015**, 153-196	0.7	
136	Gelation: the role of sugars and polyols on gelatin and agarose. *Journal of Physical Chemistry B*, **2014**, 118, 13210-6	3.4	44
135	Hydrotropy: monomer-micelle equilibrium and minimum hydrotrope concentration. *Journal of Physical Chemistry B*, **2014**, 118, 10515-24	3.4	83
134	Preferential solvation: dividing surface vs excess numbers. *Journal of Physical Chemistry B*, **2014**, 118, 3922-30	3.4	74
133	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
132	Hydration structure of CO2-absorbed 2-aminoethanol studied by neutron diffraction with the 14N/15N isotopic substitution method. *Journal of Physical Chemistry B*, **2014**, 118, 1403-10	3.4	2
131	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
130	Spatial-decomposition analysis of electrical conductivity in ionic liquid. *Journal of Chemical Physics*, **2014**, 141, 244507	3.9	11
129	2SDP-06 Interaction-Component Analysis on Protein Structure in Explicit Solvent(Biomolecular machinery driven by surrounding water,Symposium,The 52th Annual Meeting of the Biophysical Society of Japan(BSJ2014)). *Seibutsu Butsuri*, **2014**, 54, S134	0	
128	3P051 Finite-size effect on the charging free energy for protein system(01C. Protein: Property,Poster,The 52nd Annual Meeting of the Biophysical Society of Japan(BSJ2014)). *Seibutsu Butsuri*, **2014**, 54, S257	0	
127	3P132 On the Hydration Dynamics and Energetics of Alkali halide and Phosphate Ions by Dielectric Relaxation Spectroscopy and Molecular Dynamics(07. Water & Hydration & Electrolyte,Poster,The 52nd Annual Meeting of the Biophysical Society of Japan(BSJ2014)). *Seibutsu Butsuri*, **2014**, 54, S270	0	

126	Spatial-decomposition analysis of electrical conductivity in concentrated electrolyte solution. *Journal of Chemical Physics*, **2014**, 141, 044126	3.9	16
125	Effect of Rotational Couplings on Vibrational Spectrum Line Shape of the Bending Mode in Low-Density Supercritical Water: Density and Hydrogen Isotopes Dependencies. *Journal of Solution Chemistry*, **2014**, 43, 1499-1508	1.8	1
124	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
123	Interaction-component analysis of the urea effect on amino acid analogs. *Physical Chemistry Chemical Physics*, **2013**, 15, 4377-91	3.6	30
122	Molecular dynamics simulations of yeast F1-ATPase before and after 16°rotation of the □subunit. *Journal of Physical Chemistry B*, **2013**, 117, 3298-307	3.4	17
121	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
120	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
119	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
118	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
117	High-Energy X-ray Diffraction Study on the Intramolecular Structure of 2-Aminoethanol in the Liquid State. *Bulletin of the Chemical Society of Japan*, **2013**, 86, 99-103	5.1	4
116	3P164 All-atom hydration analysis of the □subunit in F1-ATPase(11. Molecular motor,Poster). *Seibutsu Butsuri*, **2013**, 53, S239	0	
115	Pathways and Kinetics of Anisole Pyrolysis Studied by NMR and Selective 13C Labeling. Heterolytic Carbon Monoxide Generation. *Bulletin of the Chemical Society of Japan*, **2012**, 85, 124-132	5.1	3
114	Interaction of naphthalene derivatives with lipids in membranes studied by the 1H-nuclear Overhauser effect and molecular dynamics simulation. *Physical Chemistry Chemical Physics*, **2012**, 14, 14049-60	3.6	6
113	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
112	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
111	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
110	Molecular dynamics study of fast dielectric relaxation of water around a molecular-sized ion. *Journal of Chemical Physics*, **2012**, 137, 224502	3.9	19
109	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

108	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
107	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
106	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
105	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
104	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
103	The effect of pressure on halothane binding to hydrated DMPC bilayers. *Molecular Physics*, **2012**, 110, 1461-1467	1.7	7
102	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
101	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
100	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
99	Distribution-function approach to free energy computation. *Journal of Chemical Physics*, **2011**, 135, 114108	3.9	13
98	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
97	Frequency-domain investigation of the ionic mobility of triflate salts in tetrahydrofuran. *Journal of Physical Chemistry B*, **2011**, 115, 12558-65	3.4	4
96	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
95	Energetic origin of proton affinity to the air/water interface. *Journal of Physical Chemistry B*, **2011**, 115, 4745-51	3.4	37
94	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
93	Development of a Quantum Chemical Method Combined with a Theory of Solutions□Free-Energy Calculation for Chemical Reactions by Condensed Phase Simulations. *Advances in Quantum Chemistry*, **2010**, 59, 283-351	1.4	2
92	Newly Designed Neutron Diffraction Cell for Fluids at High Temperatures and High Pressures. *Japanese Journal of Applied Physics*, **2010**, 49, 016602	1.4	0
91	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

90	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
89	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
88	Self-diffusion in supercritical water and benzene in high-temperature high-pressure conditions studied by NMR and dynamic solvation-shell model. *Journal of Physics: Conference Series*, **2010**, 215, 012093	0.3	4
87	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
86	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
85	Recent Advances in Studies on Organic Reactions in Water at High Temperatures and High Pressures. *Review of High Pressure Science and Technology/Koatsuryoku No Kagaku To Gijutsu*, **2010**, 20, 40-49	0	1
84	Self-diffusion coefficients for water and organic solvents in extremely low-density supercritical states. *Journal of Molecular Liquids*, **2009**, 147, 96-101	6	12
83	Water as an in situ NMR indicator for impurity acids in ionic liquids. *Analytical Chemistry*, **2009**, 81, 400-7	7.8	13
82	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
81	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
80	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
79	Hydrothermal C-C bond formation and disproportionation of acetaldehyde with formic acid. *Journal of Physical Chemistry A*, **2008**, 112, 6950-9	2.8	8
78	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
77	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
76	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
75	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
74	Free-energy change of inserting halothane into different depths of a hydrated DMPC bilayer. *Chemical Physics Letters*, **2008**, 462, 112-115	2.5	7
73	A Quantum Chemical Approach to Free Energy Calculation for Chemical Reactions in Condensed System: Combination of a Quantum Chemical Method with a Theory of Statistical Mechanics. *Challenges and Advances in Computational Chemistry and Physics*, **2008**, 455-505	0.7	3

72	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
71	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
70	Chemical equilibrium of formaldehyde and methanediol in hot water: Free-energy analysis of the solvent effect. *Journal of Molecular Liquids*, **2007**, 134, 58-63	6	27
69	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
68	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
67	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
66	Self-diffusion of supercritical water in extremely low-density region. *Journal of Chemical Physics*, **2006**, 125, 074307	3.9	33
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