Nico F A Van Der Vegt

List of Publications by Year
in descending order

167	9,841	28190 55	40881 93
papers	citations	h-index	g-index

173	173	173	8279
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Biomolecular Modeling: Goals, Problems, Perspectives. Angewandte Chemie - International Edition, 2006, 45, 4064-4092.	7.2	503
2	Validation of the 53A6 GROMOS force field. European Biophysics Journal, 2005, 34, 273-284.	1.2	443
3	What Is the Contact Angle of Water on Graphene?. Langmuir, 2013, 29, 1457-1465.	1.6	421
4	Hierarchical Modeling of Polystyrene: From Atomistic to Coarse-Grained Simulations. Macromolecules, 2006, 39, 6708-6719.	2.2	314
5	Hydration Thermodynamic Properties of Amino Acid Analogues:Â A Systematic Comparison of Biomolecular Force Fields and Water Models. Journal of Physical Chemistry B, 2006, 110, 17616-17626.	1.2	305
6	Systematic coarse-graining methods for soft matter simulations â€“ a review. Soft Matter, 2013, 9, 2108-2119.	1.2	301
7	Cation specific binding with protein surface charges. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 13296-13300.	3.3	226
8	Water-Mediated Ion Pairing: Occurrence and Relevance. Chemical Reviews, 2016, 116, 7626-7641.	23.0	195
9	Microcellular Foaming of Amorphous High-TgPolymers Using Carbon Dioxide. Macromolecules, 2001, 34, 874-884.	2.2	181
10	Open Nanoporous Morphologies from Polymeric Blends by Carbon Dioxide Foaming. Macromolecules, 2002, 35, 1738-1745.	2.2	171
11	Bicontinuous Nanoporous Polymers by Carbon Dioxide Foaming. Macromolecules, 2001, 34, 8792-8801.	2.2	169
12	Ultralow-k Dielectrics Made by Supercritical Foaming of Thin Polymer Films. Advanced Materials, 2002, 14, 1041.	11.1	164
13	Multiscale modeling of soft matter: scaling of dynamics. Physical Chemistry Chemical Physics, 2011, 13, 10412.	1.3	163
14	Comparison Between Coarseâ€Graining Models for Polymer Systems: Two Mapping Schemes for Polystyrene. Macromolecular Chemistry and Physics, 2007, 208, 2109-2120.	1.1	158
15	Coarse-Grained Polymer Melts Based on Isolated Atomistic Chains: Simulation of Polystyrene of Different Tacticities. Macromolecules, 2009, 42, 7579-7588.	2.2	148
16	Convergence of Sampling Kirkwoodâ€“Buff Integrals of Aqueous Solutions with Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2013, 9, 1347-1355.	2.3	147
17	Cation permeable membranes from blends of sulfonated poly(ether ether ketone) and poly(ether) Tj ETQq1 1 0.784314 rgBT /Overlo	4.1	133
18	Osmotic coefficients of atomistic NaCl (aq) force fields. Journal of Chemical Physics, 2006, 124, 164509.	1.2	132

#	Article	IF	Citations
19	Long time atomistic polymer trajectories from coarse grained simulations: bisphenol-A polycarbonate. Soft Matter, 2006, 2, 409-414.	1.2	123
20	Intermediate polymer to carbon gas separation membranes based on Matrimid PI. Journal of Membrane Science, 2004, 238, 93-102.	4.1	118
21	Does Urea Denature Hydrophobic Interactions?. Journal of the American Chemical Society, 2006, 128, 4948-4949.	6.6	115
22	Modeling Multibody Effects in Ionic Solutions with a Concentration Dependent Dielectric Permittivity. Physical Review Letters, 2006, 96, 147801.	2.9	110
23	How Good Are Coarseâ€Grained Polymer Models? A Comparison for Atactic Polystyrene. ChemPhysChem, 2012, 13, 3428-3439.	1.0	100
24	An Effective Force Field for Molecular Dynamics Simulations of Dimethyl Sulfoxide and Dimethyl Sulfoxideâ^'Water Mixtures. Journal of Physical Chemistry B, 2004, 108, 1436-1445.	1.2	97
25	Preparation and characterization of highly selective dense and hollow fiber asymmetric membranes based on BTDA-TDI/MDI co-polyimide. Journal of Membrane Science, 2003, 216, 195-205.	4.1	95
26	Hofmeister Ion Interactions with Model Amide Compounds. Journal of Physical Chemistry B, 2011, 115, 13781-13787.	1.2	95
27	Mechanism of Polymer Collapse in Miscible Good Solvents. Journal of Physical Chemistry B, 2015, 119, 15780-15788.	1.2	95
28	Trimethylamine N-oxide Counteracts Urea Denaturation by Inhibiting Proteinâ€“Urea Preferential Interaction. Journal of the American Chemical Society, 2018, 140, 483-492.	6.6	94
29	Bisphenol A Polycarbonate:â€‰ Entanglement Analysis from Coarse-Grained MD Simulations. Macromolecules, 2005, 38, 8078-8092.	2.2	92
30	Direct Osmolyteâ€“Macromolecule Interactions Confer Entropic Stability to Folded States. Journal of Physical Chemistry B, 2014, 118, 7327-7334.	1.2	87
31	The Hydrophobic Effect and the Role of Cosolvents. Journal of Physical Chemistry B, 2017, 121, 9986-9998.	1.2	87
32	Computer simulation studies on the solvation of aliphatic hydrocarbons in 6.9 M aqueous urea solution. Physical Chemistry Chemical Physics, 2004, 6, 697.	1.3	84
33	Carbon Dioxide Diffusion and Plasticization in Fluorinated Polyimides. Macromolecules, 2010, 43, 7813-7827.	2.2	83
34	Optimisation strategies for the preparation of bipolar membranes with reduced salt ion leakage in acidâ€“base electrodialysis. Journal of Membrane Science, 2001, 182, 13-28.	4.1	81
35	Self-assembling dipeptides: conformational sampling in solvent-free coarse-grained simulation. Physical Chemistry Chemical Physics, 2009, 11, 2077.	1.3	79
36	Free energy calculations of small molecules in dense amorphous polymers. Effect of the initial guess configuration in molecular dynamics studies. Journal of Chemical Physics, 1996, 105, 8849-8857.	1.2	78

#	Article	IF	Citations
37	Entropic Contributions in Cosolvent Binding to Hydrophobic Solutes in Water. Journal of Physical Chemistry B, 2004, 108, 1056-1064.	1.2	78
38	Conditional reversible work method for molecular coarse graining applications. Physical Chemistry Chemical Physics, 2011, 13, 10468.	1.3	77
39	Mutual Exclusion of Urea and Trimethylamine N-Oxide from Amino Acids in Mixed Solvent Environment. Journal of Physical Chemistry Letters, 2015, 6, 581-585.	2.1	72
40	Carbon molecular sieve membranes prepared from porous fiber precursor. Journal of Membrane Science, 2002, 205, 239-246.	4.1	70
41	Competing Adsorption between Hydrated Peptides and Water onto Metal Surfaces: From Electronic to Conformational Properties. Journal of the American Chemical Society, 2008, 130, 13460-13464.	6.6	68
42	Functionalized Carbon Molecular Sieve membranes containing Ag-nanoclusters. Journal of Membrane Science, 2003, 219, 47-57.	4.1	66
43	Transferability of Nonbonded Interaction Potentials for Coarse-Grained Simulations: Benzene in Water. Journal of Chemical Theory and Computation, 2010, 6, 2434-2444.	2.3	66
44	Ethylbenzene Diffusion in Polystyrene:â€‰ United Atom Atomistic/Coarse Grained Simulations and Experiments. Macromolecules, 2007, 40, 7026-7035.	2.2	64
45	Convergence of Kirkwoodâ€“Buff Integrals of Ideal and Nonideal Aqueous Solutions Using Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2018, 122, 5515-5526.	1.2	64
46	Computational Calorimetry of PNIPAM Cononsolvency in Water/Methanol Mixtures. Journal of Physical Chemistry B, 2017, 121, 7741-7748.	1.2	63
47	From Hydrophobic to Hydrophilic Solvation:â€‰ An Application to Hydration of Benzene. Journal of Chemical Theory and Computation, 2005, 1, 643-652.	2.3	62
48	Kirkwoodâ€“Buff Coarse-Grained Force Fields for Aqueous Solutions. Journal of Chemical Theory and Computation, 2012, 8, 1802-1807.	2.3	62
49	The sorption induced glass transition in amorphous glassy polymers. Journal of Chemical Physics, 1999, 110, 11061-11069.	1.2	61
50	A new force field for atomistic simulations of aqueous tertiary butanol solutions. Journal of Chemical Physics, 2005, 122, 114509.	1.2	61
51	Dual-Scale Modeling of Benzene Adsorption onto Ni(111) and Au(111) Surfaces in Explicit Water. ChemPhysChem, 2005, 6, 1866-1871.	1.0	60
52	Chemically transferable coarse-grained potentials from conditional reversible work calculations. Journal of Chemical Physics, 2012, 137, 154113.	1.2	58
53	Temperature Dependence of Gas Transport in Polymer Melts:Â Molecular Dynamics Simulations of CO2in Polyethylene. Macromolecules, 2000, 33, 3153-3160.	2.2	57
54	Understanding the Control of Mineralization by Polyelectrolyte Additives: Simulation of Preferential Binding to Calcite Surfaces. Journal of Physical Chemistry C, 2013, 117, 6904-6913.	1.5	57

#	Article	IF	Citations
55	Carbon Dioxide Solubility in Three Fluorinated Polyimides Studied by Molecular Dynamics Simulations. Macromolecules, 2010, 43, 2605-2621.	2.2	56
56	On the urea induced hydrophobic collapse of a water soluble polymer. Physical Chemistry Chemical Physics, 2015, 17, 8491-8498.	1.3	56
57	Novel open-cellular polysulfone morphologies produced with trace concentrations of solvents as pore opener. Journal of Membrane Science, 2001, 187, 181-192.	4.1	55
58	Self-assembling dipeptides: including solvent degrees of freedom in a coarse-grained model. Physical Chemistry Chemical Physics, 2009, 11, 2068.	1.3	55
59	Asymmetric Bipolar Membranes in Acidâ^'Base Electrodialysis. Industrial & Engineering Chemistry Research, 2002, 41, 579-586.	1.8	54
60	Molecular Mechanism for the Interactions of Hofmeister Cations with Macromolecules in Aqueous Solution. Journal of the American Chemical Society, 2020, 142, 19094-19100.	6.6	53
61	Transferability of Coarse Grained Potentials: Implicit Solvent Models for Hydrated Ions. Journal of Chemical Theory and Computation, 2011, 7, 1916-1927.	2.3	52
62	Introducing Memory in Coarse-Grained Molecular Simulations. Journal of Physical Chemistry B, 2021, 125, 4931-4954.	1.2	52
63	Nonadditive Ion Effects Drive Both Collapse and Swelling of Thermoresponsive Polymers in Water. Journal of the American Chemical Society, 2019, 141, 6609-6616.	6.6	51
64	Interaction of Hydrated Amino Acids with Metal Surfaces:â€‰ A Multiscale Modeling Description. Journal of Physical Chemistry C, 2007, 111, 2631-2642.	1.5	50
65	Hierarchical modeling of polymer permeation. Soft Matter, 2009, 5, 4556.	1.2	50
66	Protein Stability in TMAO and Mixed Ureaâ€“TMAO Solutions. Journal of Physical Chemistry B, 2020, 124, 6181-6197.	1.2	50
67	Energyâ€“Entropy Compensation in the Transfer of Nonpolar Solutes from Water to Cosolvent/Water Mixtures. ChemPhysChem, 2004, 5, 144-147.	1.0	49
68	Modeling of Molecular Packing and Conformation in Oligofluorenes. Journal of Physical Chemistry B, 2006, 110, 5253-5261.	1.2	48
69	Ion Pairing in Aqueous Electrolyte Solutions with Biologically Relevant Anions. Journal of Physical Chemistry B, 2011, 115, 3734-3739.	1.2	46
70	Hydrophobic Association in Mixed Ureaâ€“TMAO Solutions. Journal of Physical Chemistry Letters, 2016, 7, 3052-3059.	2.1	44
71	Ag-Functionalized Carbon Molecular-Sieve Membranes Based on Polyelectrolyte/Polyimide Blend Precursors. Advanced Functional Materials, 2005, 15, 69-75.	7.8	42
72	Unidirectional diffusion of methane in AlPO4-5. Journal of Chemical Physics, 1999, 110, 11511-11516.	1.2	41

#	Article	IF	Citations
73	Efficient sampling of solvent free energies in polymers. Journal of Chemical Physics, 1998, 109, 7578-7582.	1.2	39
74	Giant Electrorheological Effect: A Microscopic Mechanism. Physical Review Letters, 2010, 105, 046001.	2.9	39
75	Kirkwoodâ€“Buff Analysis of Liquid Mixtures in an Open Boundary Simulation. Journal of Chemical Theory and Computation, 2012, 8, 375-379.	2.3	39
76	Structural Properties of Atactic Polystyrene of Different Thermal History Obtained from a Multiscale Simulation. Macromolecules, 2009, 42, 384-391.	2.2	38
77	A Chemically Accurate Implicit-Solvent Coarse-Grained Model for Polystyrenesulfonate Solutions. Macromolecules, 2012, 45, 2551-2561.	2.2	38
78	Molecular origin of urea driven hydrophobic polymer collapse and unfolding depending on side chain chemistry. Physical Chemistry Chemical Physics, 2017, 19, 18156-18161.	1.3	37
79	Comparison of Different TMAO Force Fields and Their Impact on the Folding Equilibrium of a Hydrophobic Polymer. Journal of Physical Chemistry B, 2016, 120, 8757-8767.	1.2	36
80	Interfacial Entropy of Water on Rigid Hydrophobic Surfaces. Langmuir, 2013, 29, 9807-9813.	1.6	35
81	Fast-Growth Thermodynamic Integration:â€‰ Calculating Excess Chemical Potentials of Additive Molecules in Polymer Microstructures. Macromolecules, 2008, 41, 2283-2289.	2.2	34
82	Atomistic models of three fluorinated polyimides in the amorphous state. Journal of Polymer Science, Part B: Polymer Physics, 2009, 47, 1166-1180.	2.4	34
83	Representability and Transferability of Kirkwoodâ€“Buff Iterative Boltzmann Inversion Models for Multicomponent Aqueous Systems. Journal of Chemical Theory and Computation, 2013, 9, 5247-5256.	2.3	34
84	Transport diffusion of argon in AlPO4-5 from equilibrium molecular dynamics simulations. Journal of Chemical Physics, 2000, 113, 6875-6881.	1.2	33
85	Comparison of bipolar membranes by means of chronopotentiometry. Journal of Membrane Science, 2002, 199, 177-190.	4.1	33
86	Does an electronic continuum correction improve effective short-range ion-ion interactions in aqueous solution?. Journal of Chemical Physics, 2018, 148, 222816.	1.2	33
87	Enthalpyâ^'Entropy Compensation in the Effects of Urea on Hydrophobic Interactions. Journal of Physical Chemistry B, 2006, 110, 12852-12855.	1.2	32
88	Addressing the temperature transferability of structure based coarse graining models. Physical Chemistry Chemical Physics, 2018, 20, 6617-6628.	1.3	32
89	Nanoparticles at Biomimetic Interfaces: Combined Experimental and Simulation Study on Charged Gold Nanoparticles/Lipid Bilayer Interfaces. Journal of Physical Chemistry Letters, 2019, 10, 129-137.	2.1	30
90	Monte Carlo Simulation of Partially Confined Flexible Polymers. Macromolecules, 2002, 35, 5267-5272.	2.2	29

#	Article	IF	Citations
91	Does Preferential Adsorption Drive Cononsolvency?. Macromolecules, 2019, 52, 4131-4138.	2.2	29
92	A molecular dynamics simulation study of solvation thermodynamical quantities of gases in polymeric solvents. Journal of Membrane Science, 2002, 205, 125-139.	4.1	28
93	Novel Gas Separation Membranes Containing Covalently Bonded Fullerenes. Macromolecular Rapid Communications, 2004, 25, 1674-1678.	2.0	28
94	Cosolvent Effects on Polymer Hydration Drive Hydrophobic Collapse. Journal of Physical Chemistry B, 2018, 122, 3587-3595.	1.2	28
95	Molecular Scale Solvation in Complex Solutions. Journal of the American Chemical Society, 2019, 141, 12948-12956.	6.6	28
96	Improved Temperature Behavior of PNIPAM in Water with a Modified OPLS Model. Journal of Physical Chemistry B, 2019, 123, 3875-3883.	1.2	28
97	Cononsolvency of thermoresponsive polymers: where we are now and where we are going. Soft Matter, 2022, 18, 2884-2909.	1.2	28
98	Thermodynamics of Water Vapor Sorption in Poly(ethylene oxide) Poly(butylene terephthalate) Block Copolymers. Journal of Physical Chemistry B, 2003, 107, 13629-13635.	1.2	27
99	Bottom-up derivation of conservative and dissipative interactions for coarse-grained molecular liquids with the conditional reversible work method. Journal of Chemical Physics, 2014, 141, 224109.	1.2	27
100	Comparison of iterative inverse coarse-graining methods. European Physical Journal: Special Topics, 2016, 225, 1323-1345.	1.2	27
101	Confusing Cause and Effect:Â Energyâ^'Entropy Compensation in the Preferential Solvation of a Nonpolar Solute in Dimethyl Sulfoxide/Water Mixtures. Journal of Physical Chemistry B, 2006, 110, 12104-12112.	1.2	26
102	Thermodynamic transferability of coarse-grained potentials for polymerâ€“additive systems. Physical Chemistry Chemical Physics, 2012, 14, 11896.	1.3	26
103	Initial Electrospreading of Aqueous Electrolyte Drops. Physical Review Letters, 2013, 110, 026103.	2.9	26
104	Solid-liquid work of adhesion of coarse-grained models of n-hexane on graphene layers derived from the conditional reversible work method. Journal of Chemical Physics, 2015, 143, 243135.	1.2	25
105	Bottom-up approach to represent dynamic properties in coarse-grained molecular simulations. Journal of Chemical Physics, 2018, 149, 244114.	1.2	25
106	Orientation of liquid crystal monolayers on polyimide alignment layers: A molecular dynamics simulation study. Journal of Chemical Physics, 2001, 115, 9935-9946.	1.2	24
107	Intrinsic Conformational Preferences and Interactions in Î±-Synuclein Fibrils: Insights from Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2018, 14, 3298-3310.	2.3	24
108	Mechanism for Asymmetric Nanoscale Electrowetting of an Ionic Liquid on Graphene. Langmuir, 2016, 32, 140-150.	1.6	23

#	Article	IF	Citations
109	Modeling Solubilities of Additives in Polymer Microstructures: Single-Step Perturbation Method Based on a Soft-Cavity Reference State. Macromolecules, 2008, 41, 5055-5061.	2.2	22
110	Hierarchical modelling of polystyrene surfaces. Soft Matter, 2012, 8, 5585.	1.2	22
111	Evaluation of mapping schemes for systematic coarse graining of higher alkanes. Physical Chemistry Chemical Physics, 2017, 19, 23034-23042.	1.3	22
112	New ways to produce porous polymeric membranes by carbon dioxide foaming. Desalination, 2002, 144, 5-7.	4.0	20
113	Ionic specific effects on the structure, mechanics and interfacial softness of a polyelectrolyte brush. Faraday Discussions, 2013, 160, 297-309.	1.6	20
114	Molecular Thermodynamics of Methane Solvation in tert-Butanolâ^'Water Mixtures. Journal of Chemical Theory and Computation, 2007, 3, 194-200.	2.3	19
115	Transferability of Local Density-Assisted Implicit Solvation Models for Homogeneous Fluid Mixtures. Journal of Chemical Theory and Computation, 2019, 15, 2881-2895.	2.3	19
116	Enthalpyâ€“Entropy of Cation Association with the Acetate Anion in Water. Journal of Chemical Theory and Computation, 2012, 8, 3804-3809.	2.3	18
117	Phase Equilibria Modeling with Systematically Coarse-Grained Modelsâ€”A Comparative Study on State Point Transferability. Journal of Physical Chemistry B, 2019, 123, 504-515.	1.2	18
118	Solvent Reorganization Contributions in Solute Transfer Thermodynamics:â€‰ Inferences from the Solvent Equation of State. Journal of Physical Chemistry B, 2007, 111, 7836-7842.	1.2	17
119	Equilibration and Deformation of Amorphous Polystyrene: Scaleâ€jumping Simulational Approach. Macromolecular Theory and Simulations, 2008, 17, 290-300.	0.6	17
120	Basis of Solubility versusT_CCorrelations in Polymeric Gas Separation Membranes. Macromolecules, 2010, 43, 1473-1479.	2.2	17
121	Preferential Solvation of Triglycine in Aqueous Urea: An Open Boundary Simulation Approach. Journal of Chemical Theory and Computation, 2012, 8, 3536-3541.	2.3	17
122	Interfacial Tension Does Not Drive Asymmetric Nanoscale Electrowetting on Graphene. Langmuir, 2015, 31, 4686-4695.	1.6	17
123	Predictive Modeling of Phenol Chemical Potentials in Molten Bisphenol Aâ^'Polycarbonate over a Broad Temperature Range. Macromolecules, 2008, 41, 7281-7283.	2.2	16
124	Solvation thermodynamics of amino acid side chains on a short peptide backbone. Journal of Chemical Physics, 2015, 142, 144502.	1.2	16
125	An interplay of excluded-volume and polymerâ€“(co)solvent attractive interactions regulates polymer collapse in mixed solvents. Journal of Chemical Physics, 2021, 154, 134903.	1.2	16
126	Porous Monofilaments by Continuous Solid-State Foaming. Industrial & Engineering Chemistry Research, 2002, 41, 1195-1204.	1.8	15

#	Article	IF	Citations
127	Molecular Simulation Via Connectivityâ€altering Monte Carlo and Scaleâ€jumping Methods: Application to Amorphous Polystyrene. Macromolecular Theory and Simulations, 2008, 17, 393-402.	0.6	15
128	Molecular Simulation Study on Hofmeister Cations and the Aqueous Solubility of Benzene. Journal of Physical Chemistry B, 2014, 118, 5331-5339.	1.2	15
129	Modelling moleculeâ€“surface interactionsâ€”an automated quantum-classical approach using a genetic algorithm. Physical Chemistry Chemical Physics, 2011, 13, 10577.	1.3	14
130	Development of Classical Moleculeâ€“Surface Interaction Potentials Based on Density Functional Theory Calculations: Investigation of Force Field Representability. Journal of Physical Chemistry C, 2012, 116, 19781-19788.	1.5	14
131	Comment on â€œRelating side chain organization of PNIPAm with its conformation in aqueous methanolâ€• by D. Mukherji, M. Wagner, M. D. Watson, S. Winzen, T. E. de Oliveira, C. M. Marques and K. Kremer, Soft Matter, 2016, 12, 7995. Soft Matter, 2017, 13, 2289-2291.	1.2	14
132	A cosolvent surfactant mechanism affects polymer collapse in miscible good solvents. Communications Chemistry, 2020, 3, .	2.0	14
133	Length-Scale Effects in Hydrophobic Polymer Collapse Transitions. Journal of Physical Chemistry B, 2021, 125, 5191-5199.	1.2	12
134	Cross-correlation corrected friction in (generalized) Langevin models. Journal of Chemical Physics, 2021, 154, 191102.	1.2	12
135	Peptide Backbone Effect on Hydration Free Energies of Amino Acid Side Chains. Journal of Physical Chemistry B, 2014, 118, 13162-13168.	1.2	11
136	How does low-molecular-weight polystyrene dissolve: osmotic swelling vs. surface dissolution. Soft Matter, 2014, 10, 9059-9064.	1.2	11
137	Conditional Reversible Work Coarse-Grained Models of Molecular Liquids with Coulomb Electrostatics â€“ A Proof of Concept Study on Weakly Polar Organic Molecules. Journal of Chemical Theory and Computation, 2017, 13, 6158-6166.	2.3	11
138	Where Lennard-Jones Potentials Fail: Iterative Optimization of Ionâ€“Water Pair Potentials Based on Ab Initio Molecular Dynamics Data. Journal of Physical Chemistry Letters, 2022, 13, 3712-3717.	2.1	10
139	Polymer intrusion into narrow pores at the interface between a poor solvent and adsorbing and non-adsorbing surfaces. Polymer, 2004, 45, 3027-3036.	1.8	9
140	Multiscale Approaches and Perspectives to Modeling Aqueous Electrolytes and Polyelectrolytes. Topics in Current Chemistry, 2011, 307, 251-294.	4.0	9
141	Understanding the influence of capillary waves on solvation at the liquid-vapor interface. Journal of Chemical Physics, 2016, 144, 114111.	1.2	9
142	Contact Ion Pairs in the Bulk Affect Anion Interactions with Poly(N-isopropylacrylamide). Journal of Physical Chemistry B, 2021, 125, 680-688.	1.2	9
143	Solvent-averaged potentials for alkali-, earth alkali-, and alkylammonium halide aqueous solutions. Journal of Chemical Physics, 2007, 127, 234508.	1.2	8
144	Vortex formation in coalescence of droplets with a reservoir using molecular dynamics simulations. Journal of Colloid and Interface Science, 2016, 479, 189-198.	5.0	8

#	Article	IF	Citations
145	Application of the 2PT model to understanding entropy change in molecular coarse-graining. Soft Materials, 2020, 18, 274-289.	0.8	8
146	Pressure, Peptides, and a Piezolyte: Structural Analysis of the Effects of Pressure and Trimethylamine-‹i›N‹/i›-oxide on the Peptide Solvation Shell. Journal of Physical Chemistry B, 2020, 124, 6508-6519.	1.2	8
147	Nonadditive ion effects on the coilâ€“globule equilibrium of PNIPAM: a computer simulation study. Physical Chemistry Chemical Physics, 2022, 24, 10346-10355.	1.3	8
148	Conditional Reversible Work Coarse-Grained Models with Explicit Electrostaticsâ€”An Application to Butylmethylimidazolium Ionic Liquids. Journal of Chemical Theory and Computation, 2019, 15, 1187-1198.	2.3	7
149	Characterizing Polymer Hydration Shell Compressibilities with the Small-System Method. Nanomaterials, 2020, 10, 1460.	1.9	7
150	Cross-correlation corrected friction in generalized Langevin models: Application to the continuous Asakuraâ€“Oosawa model. Journal of Chemical Physics, 2022, 157, .	1.2	7
151	1-Butanol absorption in poly(styrene-divinylbenzene) ion exchange resins for catalysis. Soft Matter, 2015, 11, 9144-9149.	1.2	6
152	Using Grand Canonical Monte Carlo Simulations to Understand the Role of Interfacial Fluctuations on Solvation at the Waterâ€“Vapor Interface. Journal of Physical Chemistry B, 2016, 120, 9697-9707.	1.2	6
153	Iterative integral equation methods for structural coarse-graining. Journal of Chemical Physics, 2021, 154, 084118.	1.2	6
154	Coarse-grained model of a nanoscale-segregated ionic liquid for simulations of low-temperature structure and dynamics. Journal of Physics Condensed Matter, 2021, 33, 204002.	0.7	6
155	Monte Carlo Calculations of Polymer Adsorption at the Entrance of Cylindrical Pores in Flat Adsorbing Surfaces. Soft Materials, 2003, 1, 295-312.	0.8	5
156	Grand challenges in quantumâ€classical modeling of moleculeâ€“surface interactions. Journal of Computational Chemistry, 2013, 34, 1177-1188.	1.5	5
157	Study of Hydrophobic Clustering in Partially Sulfonated Polystyrene Solutions with a Systematic Coarse-Grained Model. Macromolecules, 2016, 49, 7571-7580.	2.2	5
158	Structure-Based Coarse- and Fine-Graining in Soft Matter Simulations. , 2008, , .		5
159	Small-to-large length scale transition of TMAO interaction with hydrophobic solutes. Physical Chemistry Chemical Physics, 2022, 24, 2080-2087.	1.3	5
160	Interaction of Water with N,Nâ€²â€²1,2-Ethanediyl-bis(6-hydroxy-hexanamide) Crystals: A Simulation Study. Journal of Physical Chemistry B, 2009, 113, 627-631.	1.2	3
161	Relative entropy indicates an ideal concentration for structure-based coarse graining of binary mixtures. Physical Review E, 2019, 99, 053308.	0.8	3
162	Direct Calculation of Entropic Components in Cohesive Interaction Free Energies. Journal of Physical Chemistry B, 2021, 125, 11026-11035.	1.2	2

#	Article	IF	Citations
163	MICROSCOPIC MECHANISM OF THE GIANT ELECTRORHEOLOGICAL EFFECT. International Journal of Modern Physics B, 2011, 25, 897-903.	1.0	1
164	Temperature induced change of TMAO effects on hydrophobic hydration. Journal of Chemical Physics, 2022, 156, 184501.	1.2	1
165	Energy-Entropy Compensation in the Transfer of Nonpolar Solutes from Water to Cosolvent/Water Mixtures. ChemPhysChem, 2005, 6, 1010-1010.	1.0	0
166	MICROSCOPIC MECHANISM OF THE GIANT ELECTRORHEOLOGICAL EFFECT. , 2011, , .		0
167	Solvation Shell Thermodynamics of Extended Hydrophobic Solutes in Mixed Solvents. Journal of Chemical Physics, 2022, 156, 164901.	1.2	0