Nico F A Van Der Vegt

List of Publications by Year
in descending order

167 papers	9,841 citations	32410 55 h-index	46524 93 g-index

173 all docs	173 docs citations	173 times ranked	9503 citing authors

#	Article	IF	Citations
1	Small-to-large length scale transition of TMAO interaction with hydrophobic solutes. Physical Chemistry Chemical Physics, 2022, 24, 2080-2087.	1.3	5
2	Cononsolvency of thermoresponsive polymers: where we are now and where we are going. Soft Matter, 2022, 18, 2884-2909.	1.2	28
3	Solvation Shell Thermodynamics of Extended Hydrophobic Solutes in Mixed Solvents. Journal of Chemical Physics, 2022, 156, 164901.	1.2	0
4	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
5	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
6	Temperature induced change of TMAO effects on hydrophobic hydration. Journal of Chemical Physics, 2022, 156, 184501.	1.2	1
7	Cross-correlation corrected friction in generalized Langevin models: Application to the continuous Asakuraâ€“Oosawa model. Journal of Chemical Physics, 2022, 157, .	1.2	7
8	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
9	Iterative integral equation methods for structural coarse-graining. Journal of Chemical Physics, 2021, 154, 084118.	1.2	6
10	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
11	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
12	Length-Scale Effects in Hydrophobic Polymer Collapse Transitions. Journal of Physical Chemistry B, 2021, 125, 5191-5199.	1.2	12
13	Introducing Memory in Coarse-Grained Molecular Simulations. Journal of Physical Chemistry B, 2021, 125, 4931-4954.	1.2	52
14	Cross-correlation corrected friction in (generalized) Langevin models. Journal of Chemical Physics, 2021, 154, 191102.	1.2	12
15	Direct Calculation of Entropic Components in Cohesive Interaction Free Energies. Journal of Physical Chemistry B, 2021, 125, 11026-11035.	1.2	2
16	Characterizing Polymer Hydration Shell Compressibilities with the Small-System Method. Nanomaterials, 2020, 10, 1460.	1.9	7
17	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
18	A cosolvent surfactant mechanism affects polymer collapse in miscible good solvents. Communications Chemistry, 2020, 3, .	2.0	14

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19	Protein Stability in TMAO and Mixed Ureaâ€“TMAO Solutions. Journal of Physical Chemistry B, 2020, 124, 6181-6197.	1.2	50
20	Application of the 2PT model to understanding entropy change in molecular coarse-graining. Soft Materials, 2020, 18, 274-289.	0.8	8
21	Pressure, Peptides, and a Piezolyte: Structural Analysis of the Effects of Pressure and Trimethylamine-N-oxide on the Peptide Solvation Shell. Journal of Physical Chemistry B, 2020, 124, 6508-6519.	1.2	8
22	Molecular Scale Solvation in Complex Solutions. Journal of the American Chemical Society, 2019, 141, 12948-12956.	6.6	28
23	Does Preferential Adsorption Drive Cononsolvency?. Macromolecules, 2019, 52, 4131-4138.	2.2	29
24	Relative entropy indicates an ideal concentration for structure-based coarse graining of binary mixtures. Physical Review E, 2019, 99, 053308.	0.8	3
25	Improved Temperature Behavior of PNIPAM in Water with a Modified OPLS Model. Journal of Physical Chemistry B, 2019, 123, 3875-3883.	1.2	28
26	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
27	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
28	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
29	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
30	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
31	Cosolvent Effects on Polymer Hydration Drive Hydrophobic Collapse. Journal of Physical Chemistry B, 2018, 122, 3587-3595.	1.2	28
32	Addressing the temperature transferability of structure based coarse graining models. Physical Chemistry Chemical Physics, 2018, 20, 6617-6628.	1.3	32
33	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
34	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
35	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
36	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

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37	Bottom-up approach to represent dynamic properties in coarse-grained molecular simulations. Journal of Chemical Physics, 2018, 149, 244114.	1.2	25
38	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
39	Evaluation of mapping schemes for systematic coarse graining of higher alkanes. Physical Chemistry Chemical Physics, 2017, 19, 23034-23042.	1.3	22
40	The Hydrophobic Effect and the Role of Cosolvents. Journal of Physical Chemistry B, 2017, 121, 9986-9998.	1.2	87
41	Computational Calorimetry of PNIPAM Cononsolvency in Water/Methanol Mixtures. Journal of Physical Chemistry B, 2017, 121, 7741-7748.	1.2	63
42	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
43	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
44	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
45	Understanding the influence of capillary waves on solvation at the liquid-vapor interface. Journal of Chemical Physics, 2016, 144, 114111.	1.2	9
46	Water-Mediated Ion Pairing: Occurrence and Relevance. Chemical Reviews, 2016, 116, 7626-7641.	23.0	195
47	Study of Hydrophobic Clustering in Partially Sulfonated Polystyrene Solutions with a Systematic Coarse-Grained Model. Macromolecules, 2016, 49, 7571-7580.	2.2	5
48	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
49	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
50	Hydrophobic Association in Mixed Ureaâ€“TMAO Solutions. Journal of Physical Chemistry Letters, 2016, 7, 3052-3059.	2.1	44
51	Comparison of iterative inverse coarse-graining methods. European Physical Journal: Special Topics, 2016, 225, 1323-1345.	1.2	27
52	Mechanism for Asymmetric Nanoscale Electrowetting of an Ionic Liquid on Graphene. Langmuir, 2016, 32, 140-150.	1.6	23
53	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
54	Mechanism of Polymer Collapse in Miscible Good Solvents. Journal of Physical Chemistry B, 2015, 119, 15780-15788.	1.2	95

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55	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
56	On the urea induced hydrophobic collapse of a water soluble polymer. Physical Chemistry Chemical Physics, 2015, 17, 8491-8498.	1.3	56
57	Interfacial Tension Does Not Drive Asymmetric Nanoscale Electrowetting on Graphene. Langmuir, 2015, 31, 4686-4695.	1.6	17
58	Solvation thermodynamics of amino acid side chains on a short peptide backbone. Journal of Chemical Physics, 2015, 142, 144502.	1.2	16
59	1-Butanol absorption in poly(styrene-divinylbenzene) ion exchange resins for catalysis. Soft Matter, 2015, 11, 9144-9149.	1.2	6
60	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
61	Peptide Backbone Effect on Hydration Free Energies of Amino Acid Side Chains. Journal of Physical Chemistry B, 2014, 118, 13162-13168.	1.2	11
62	How does low-molecular-weight polystyrene dissolve: osmotic swelling vs. surface dissolution. Soft Matter, 2014, 10, 9059-9064.	1.2	11
63	Direct Osmolyteâ€“Macromolecule Interactions Confer Entropic Stability to Folded States. Journal of Physical Chemistry B, 2014, 118, 7327-7334.	1.2	87
64	Molecular Simulation Study on Hofmeister Cations and the Aqueous Solubility of Benzene. Journal of Physical Chemistry B, 2014, 118, 5331-5339.	1.2	15
65	Interfacial Entropy of Water on Rigid Hydrophobic Surfaces. Langmuir, 2013, 29, 9807-9813.	1.6	35
66	Initial Electrospreading of Aqueous Electrolyte Drops. Physical Review Letters, 2013, 110, 026103.	2.9	26
67	What Is the Contact Angle of Water on Graphene?. Langmuir, 2013, 29, 1457-1465.	1.6	421
68	Systematic coarse-graining methods for soft matter simulations â€“ a review. Soft Matter, 2013, 9, 2108-2119.	1.2	301
69	Ionic specific effects on the structure, mechanics and interfacial softness of a polyelectrolyte brush. Faraday Discussions, 2013, 160, 297-309.	1.6	20
70	Grand challenges in quantumâ€classical modeling of moleculeâ€“surface interactions. Journal of Computational Chemistry, 2013, 34, 1177-1188.	1.5	5
71	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
72	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

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73	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
74	Chemically transferable coarse-grained potentials from conditional reversible work calculations. Journal of Chemical Physics, 2012, 137, 154113.	1.2	58
75	Enthalpyâ€“Entropy of Cation Association with the Acetate Anion in Water. Journal of Chemical Theory and Computation, 2012, 8, 3804-3809.	2.3	18
76	Kirkwoodâ€“Buff Analysis of Liquid Mixtures in an Open Boundary Simulation. Journal of Chemical Theory and Computation, 2012, 8, 375-379.	2.3	39
77	Thermodynamic transferability of coarse-grained potentials for polymerâ€“additive systems. Physical Chemistry Chemical Physics, 2012, 14, 11896.	1.3	26
78	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
79	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
80	A Chemically Accurate Implicit-Solvent Coarse-Grained Model for Polystyrenesulfonate Solutions. Macromolecules, 2012, 45, 2551-2561.	2.2	38
81	Hierarchical modelling of polystyrene surfaces. Soft Matter, 2012, 8, 5585.	1.2	22
82	Kirkwoodâ€“Buff Coarse-Grained Force Fields for Aqueous Solutions. Journal of Chemical Theory and Computation, 2012, 8, 1802-1807.	2.3	62
83	How Good Are Coarseâ€Grained Polymer Models? A Comparison for Atactic Polystyrene. ChemPhysChem, 2012, 13, 3428-3439.	1.0	100
84	Modelling moleculeâ€“surface interactionsâ€”an automated quantum-classical approach using a genetic algorithm. Physical Chemistry Chemical Physics, 2011, 13, 10577.	1.3	14
85	Conditional reversible work method for molecular coarse graining applications. Physical Chemistry Chemical Physics, 2011, 13, 10468.	1.3	77
86	Hofmeister Ion Interactions with Model Amide Compounds. Journal of Physical Chemistry B, 2011, 115, 13781-13787.	1.2	95
87	Multiscale modeling of soft matter: scaling of dynamics. Physical Chemistry Chemical Physics, 2011, 13, 10412.	1.3	163
88	Transferability of Coarse Grained Potentials: Implicit Solvent Models for Hydrated Ions. Journal of Chemical Theory and Computation, 2011, 7, 1916-1927.	2.3	52
89	Ion Pairing in Aqueous Electrolyte Solutions with Biologically Relevant Anions. Journal of Physical Chemistry B, 2011, 115, 3734-3739.	1.2	46
90	MICROSCOPIC MECHANISM OF THE GIANT ELECTRORHEOLOGICAL EFFECT. International Journal of Modern Physics B, 2011, 25, 897-903.	1.0	1

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91	Multiscale Approaches and Perspectives to Modeling Aqueous Electrolytes and Polyelectrolytes. Topics in Current Chemistry, 2011, 307, 251-294.	4.0	9
92	MICROSCOPIC MECHANISM OF THE GIANT ELECTRORHEOLOGICAL EFFECT. , 2011, , .		0
93	Carbon Dioxide Diffusion and Plasticization in Fluorinated Polyimides. Macromolecules, 2010, 43, 7813-7827.	2.2	83
94	Giant Electrorheological Effect: A Microscopic Mechanism. Physical Review Letters, 2010, 105, 046001.	2.9	39
95	Basis of Solubility versusT_CCorrelations in Polymeric Gas Separation Membranes. Macromolecules, 2010, 43, 1473-1479.	2.2	17
96	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
97	Carbon Dioxide Solubility in Three Fluorinated Polyimides Studied by Molecular Dynamics Simulations. Macromolecules, 2010, 43, 2605-2621.	2.2	56
98	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
99	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
100	Interaction of Water with N,Nâ€²â˜’1,2-Ethanediyl-bis(6-hydroxy-hexanamide) Crystals: A Simulation Study. Journal of Physical Chemistry B, 2009, 113, 627-631.	1.2	3
101	Coarse-Grained Polymer Melts Based on Isolated Atomistic Chains: Simulation of Polystyrene of Different Tacticities. Macromolecules, 2009, 42, 7579-7588.	2.2	148
102	Structural Properties of Atactic Polystyrene of Different Thermal History Obtained from a Multiscale Simulation. Macromolecules, 2009, 42, 384-391.	2.2	38
103	Self-assembling dipeptides: conformational sampling in solvent-free coarse-grained simulation. Physical Chemistry Chemical Physics, 2009, 11, 2077.	1.3	79
104	Self-assembling dipeptides: including solvent degrees of freedom in a coarse-grained model. Physical Chemistry Chemical Physics, 2009, 11, 2068.	1.3	55
105	Hierarchical modeling of polymer permeation. Soft Matter, 2009, 5, 4556.	1.2	50
106	Equilibration and Deformation of Amorphous Polystyrene: Scaleâ€jumping Simulational Approach. Macromolecular Theory and Simulations, 2008, 17, 290-300.	0.6	17
107	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
108	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

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109	Predictive Modeling of Phenol Chemical Potentials in Molten Bisphenol Aâ˜Polycarbonate over a Broad Temperature Range. Macromolecules, 2008, 41, 7281-7283.	2.2	16
110	Fast-Growth Thermodynamic Integration:â€‰ Calculating Excess Chemical Potentials of Additive Molecules in Polymer Microstructures. Macromolecules, 2008, 41, 2283-2289.	2.2	34
111	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
112	Structure-Based Coarse- and Fine-Graining in Soft Matter Simulations. , 2008, , .		5
113	Solvent-averaged potentials for alkali-, earth alkali-, and alkylammonium halide aqueous solutions. Journal of Chemical Physics, 2007, 127, 234508.	1.2	8
114	Ethylbenzene Diffusion in Polystyrene:â€‰ United Atom Atomistic/Coarse Grained Simulations and Experiments. Macromolecules, 2007, 40, 7026-7035.	2.2	64
115	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
116	Molecular Thermodynamics of Methane Solvation in tert-Butanolâ˜Water Mixtures. Journal of Chemical Theory and Computation, 2007, 3, 194-200.	2.3	19
117	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
118	Comparison Between Coarseâ€Graining Models for Polymer Systems: Two Mapping Schemes for Polystyrene. Macromolecular Chemistry and Physics, 2007, 208, 2109-2120.	1.1	158
119	Modeling Multibody Effects in Ionic Solutions with a Concentration Dependent Dielectric Permittivity. Physical Review Letters, 2006, 96, 147801.	2.9	110
120	Osmotic coefficients of atomistic NaCl (aq) force fields. Journal of Chemical Physics, 2006, 124, 164509.	1.2	132
121	Long time atomistic polymer trajectories from coarse grained simulations: bisphenol-A polycarbonate. Soft Matter, 2006, 2, 409-414.	1.2	123
122	Does Urea Denature Hydrophobic Interactions?. Journal of the American Chemical Society, 2006, 128, 4948-4949.	6.6	115
123	Enthalpyâ˜Entropy Compensation in the Effects of Urea on Hydrophobic Interactions. Journal of Physical Chemistry B, 2006, 110, 12852-12855.	1.2	32
124	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
125	Modeling of Molecular Packing and Conformation in Oligofluorenes. Journal of Physical Chemistry B, 2006, 110, 5253-5261.	1.2	48
126	Hierarchical Modeling of Polystyrene: From Atomistic to Coarse-Grained Simulations. Macromolecules, 2006, 39, 6708-6719.	2.2	314

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127	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
128	Biomolecular Modeling: Goals, Problems, Perspectives. Angewandte Chemie - International Edition, 2006, 45, 4064-4092.	7.2	503
129	Dual-Scale Modeling of Benzene Adsorption onto Ni(111) and Au(111) Surfaces in Explicit Water. ChemPhysChem, 2005, 6, 1866-1871.	1.0	60
130	Energy-Entropy Compensation in the Transfer of Nonpolar Solutes from Water to Cosolvent/Water Mixtures. ChemPhysChem, 2005, 6, 1010-1010.	1.0	0
131	Ag-Functionalized Carbon Molecular-Sieve Membranes Based on Polyelectrolyte/Polyimide Blend Precursors. Advanced Functional Materials, 2005, 15, 69-75.	7.8	42
132	Validation of the 53A6 GROMOS force field. European Biophysics Journal, 2005, 34, 273-284.	1.2	443
133	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
134	Bisphenol A Polycarbonate:â€‰ Entanglement Analysis from Coarse-Grained MD Simulations. Macromolecules, 2005, 38, 8078-8092.	2.2	92
135	A new force field for atomistic simulations of aqueous tertiary butanol solutions. Journal of Chemical Physics, 2005, 122, 114509.	1.2	61
136	Energyâ€“Entropy Compensation in the Transfer of Nonpolar Solutes from Water to Cosolvent/Water Mixtures. ChemPhysChem, 2004, 5, 144-147.	1.0	49
137	Novel Gas Separation Membranes Containing Covalently Bonded Fullerenes. Macromolecular Rapid Communications, 2004, 25, 1674-1678.	2.0	28
138	Intermediate polymer to carbon gas separation membranes based on Matrimid PI. Journal of Membrane Science, 2004, 238, 93-102.	4.1	118
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	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
141	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
142	Entropic Contributions in Cosolvent Binding to Hydrophobic Solutes in Water. Journal of Physical Chemistry B, 2004, 108, 1056-1064.	1.2	78
143	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
144	Functionalized Carbon Molecular Sieve membranes containing Ag-nanoclusters. Journal of Membrane Science, 2003, 219, 47-57.	4.1	66

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145	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
146	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
147	Porous Monofilaments by Continuous Solid-State Foaming. Industrial & Engineering Chemistry Research, 2002, 41, 1195-1204.	1.8	15
148	Monte Carlo Simulation of Partially Confined Flexible Polymers. Macromolecules, 2002, 35, 5267-5272.	2.2	29
149	Open Nanoporous Morphologies from Polymeric Blends by Carbon Dioxide Foaming. Macromolecules, 2002, 35, 1738-1745.	2.2	171
150	Asymmetric Bipolar Membranes in Acidâ^'Base Electrodialysis. Industrial & Engineering Chemistry Research, 2002, 41, 579-586.	1.8	54
151	Ultralow-k Dielectrics Made by Supercritical Foaming of Thin Polymer Films. Advanced Materials, 2002, 14, 1041.	11.1	164
152	Cation permeable membranes from blends of sulfonated poly(ether ether ketone) and poly(ether) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50	4.1	133
153	Comparison of bipolar membranes by means of chronopotentiometry. Journal of Membrane Science, 2002, 199, 177-190.	4.1	33
154	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
155	Carbon molecular sieve membranes prepared from porous fiber precursor. Journal of Membrane Science, 2002, 205, 239-246.	4.1	70
156	New ways to produce porous polymeric membranes by carbon dioxide foaming. Desalination, 2002, 144, 5-7.	4.0	20
157	Microcellular Foaming of Amorphous High-TgPolymers Using Carbon Dioxide. Macromolecules, 2001, 34, 874-884.	2.2	181
158	Bicontinuous Nanoporous Polymers by Carbon Dioxide Foaming. Macromolecules, 2001, 34, 8792-8801.	2.2	169
159	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
160	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
161	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
162	Transport diffusion of argon in AlPO4-5 from equilibrium molecular dynamics simulations. Journal of Chemical Physics, 2000, 113, 6875-6881.	1.2	33

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163	Temperature Dependence of Gas Transport in Polymer Melts:Â Molecular Dynamics Simulations of CO2in Polyethylene. Macromolecules, 2000, 33, 3153-3160.	2.2	57
164	Unidirectional diffusion of methane in AlPO4-5. Journal of Chemical Physics, 1999, 110, 11511-11516.	1.2	41
165	The sorption induced glass transition in amorphous glassy polymers. Journal of Chemical Physics, 1999, 110, 11061-11069.	1.2	61
166	Efficient sampling of solvent free energies in polymers. Journal of Chemical Physics, 1998, 109, 7578-7582.	1.2	39
167	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