Peter T Cummings

List of Publications by Year
in descending order

469	19,206	10956 71	24179 110
papers	citations	h-index	g-index

484	484	484	12990
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Tumor Morphology and Phenotypic Evolution Driven by Selective Pressure from the Microenvironment. Cell, 2006, 127, 905-915.	13.5	714
2	Three-dimensional tracking of motile bacteria near a solid planar surface.. Proceedings of the National Academy of Sciences of the United States of America, 1995, 92, 6195-6199.	3.3	328
3	Supercapacitor Capacitance Exhibits Oscillatory Behavior as a Function of Nanopore Size. Journal of Physical Chemistry Letters, 2011, 2, 2859-2864.	2.1	316
4	Electric Double Layer at the Rutile (110) Surface. 1. Structure of Surfaces and Interfacial Water from Molecular Dynamics by Use of ab Initio Potentials. Journal of Physical Chemistry B, 2004, 108, 12049-12060.	1.2	272
5	Improvement of Quality in Publication of Experimental Thermophysical Property Data: Challenges, Assessment Tools, Global Implementation, and Online Support. Journal of Chemical & Engineering Data, 2013, 58, 2699-2716.	1.0	236
6	Water in carbon nanotubes: Adsorption isotherms and thermodynamic properties from molecular simulation. Journal of Chemical Physics, 2005, 122, 234712.	1.2	225
7	Water Adsorption in Carbon-Slit Nanopores. Langmuir, 2003, 19, 8583-8591.	1.6	212
8	From dimer to condensed phases at extreme conditions: Accurate predictions of the properties of water by a Gaussian charge polarizable model. Journal of Chemical Physics, 2005, 122, 244511.	1.2	202
9	Characterization of Titanium Dioxide Nanoparticles Using Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2005, 109, 15243-15249.	1.2	197
10	Simulation of supercritical water and of supercritical aqueous solutions. Journal of Chemical Physics, 1991, 94, 5606-5621.	1.2	188
11	Simulations of the Quartz(101Ì…1)/Water Interface: A Comparison of Classical Force Fields, Ab Initio Molecular Dynamics, and X-ray Reflectivity Experiments. Journal of Physical Chemistry C, 2011, 115, 2076-2088.	1.5	183
12	Computational Insights into Materials and Interfaces for Capacitive Energy Storage. Advanced Science, 2017, 4, 1700059.	5.6	176
13	Quantitative comparison and optimization of methods for evaluating the chemical potential by molecular simulation. Molecular Physics, 1997, 92, 973-996.	0.8	175
14	Solute-induced effects on the structure and thermodynamics of infinitely dilute mixtures. AICHE Journal, 1994, 40, 1558-1573.	1.8	172
15	Oscillatory Behavior of Double-Walled Nanotubes under Extension:â€‰ A Simple Nanoscale Damped Spring. Nano Letters, 2003, 3, 1001-1005.	4.5	171
16	Fluidity of Hydration Layers Nanoconfined between Mica Surfaces. Physical Review Letters, 2005, 94, 026101.	2.9	169
17	Process optimization via simulated annealing: Application to network design. AICHE Journal, 1989, 35, 725-736.	1.8	167
18	Molecular simulation of water along the liquidâ€“vapor coexistence curve from 25â€‰Â°C to the critical point. Journal of Chemical Physics, 1990, 93, 7355-7359.	1.2	160

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19	Engineering a simple polarizable model for the molecular simulation of water applicable over wide ranges of state conditions. Journal of Chemical Physics, 1996, 105, 8274-8281.	1.2	151
20	Nanoscale Perturbations of Room Temperature Ionic Liquid Structure at Charged and Uncharged Interfaces. ACS Nano, 2012, 6, 9818-9827.	7.3	151
21	Molecular simulations of liquid-liquid interfacial properties: Waterâ€“n-alkane and water-methanolâ€“n-alkane systems. Physical Review E, 2003, 67, 011603.	0.8	149
22	Statistical mechanical models of chemical reactions. Molecular Physics, 1984, 51, 253-287.	0.8	147
23	Bias-Dependent Molecular-Level Structure of Electrical Double Layer in Ionic Liquid on Graphite. Nano Letters, 2013, 13, 5954-5960.	4.5	142
24	Na+â€“Clâ¯ion pair association in supercritical water. Journal of Chemical Physics, 1995, 103, 9379-9387.	1.2	141
25	Molecular Dynamics Simulation of Titanium Dioxide Nanoparticle Sintering. Journal of Physical Chemistry B, 2005, 109, 24280-24287.	1.2	141
26	Comparison of shear flow of hexadecane in a confined geometry and in bulk. Journal of Chemical Physics, 1997, 106, 7303-7314.	1.2	139
27	Molecular simulation of the transition from liquidlike to solidlike behavior in complex fluids confined to nanoscale gaps. Journal of Chemical Physics, 2001, 114, 7189-7195.	1.2	136
28	Dynamics and Structure of Hydration Water on Rutile and Cassiterite Nanopowders Studied by Quasielastic Neutron Scattering and Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2007, 111, 4328-4341.	1.5	132
29	Continuous transition from double-layer to Faradaic charge storage in confined electrolytes. Nature Energy, 2022, 7, 222-228.	19.8	130
30	Microstructure of Ambient and Supercritical Water. Direct Comparison between Simulation and Neutron Scattering Experiments. The Journal of Physical Chemistry, 1996, 100, 1309-1316.	2.9	129
31	C60 Binds to and Deforms Nucleotides. Biophysical Journal, 2005, 89, 3856-3862.	0.2	129
32	Electric Double Layer at the Rutile (110) Surface. 2. Adsorption of Ions from Molecular Dynamics and X-ray Experiments. Journal of Physical Chemistry B, 2004, 108, 12061-12072.	1.2	127
33	Curvature Effect on the Capacitance of Electric Double Layers at Ionic Liquid/Onion-Like Carbon Interfaces. Journal of Chemical Theory and Computation, 2012, 8, 1058-1063.	2.3	125
34	Molecular Insights into Carbon Supercapacitors Based on Room-Temperature Ionic Liquids. Journal of Physical Chemistry Letters, 2013, 4, 3367-3376.	2.1	125
35	Comparison of Nonequilibrium Molecular Dynamics with Experimental Measurements in the Nonlinear Shear-Thinning Regime. Physical Review Letters, 2002, 88, 058302.	2.9	124
36	Molecular dynamics simulations of the rheology of normal decane, hexadecane, and tetracosane. Journal of Chemical Physics, 1996, 105, 1214-1220.	1.2	123

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37	Hydrogen bonding in supercritical water. Journal of Chemical Physics, 1994, 101, 4466-4469.	1.2	121
38	Alkyl Chain Length and Temperature Effects on Structural Properties of Pyrrolidinium-Based Ionic Liquids: A Combined Atomistic Simulation and Small-Angle X-ray Scattering Study. Journal of Physical Chemistry Letters, 2012, 3, 125-130.	2.1	121
39	Nonequilibrium molecular dynamics approaches to transport properties and non-Newtonian fluid rheology. Industrial & Engineering Chemistry Research, 1992, 31, 1237-1252.	1.8	116
40	Interaction site models for molecular fluids. Molecular Physics, 1982, 46, 383-426.	0.8	111
41	Supercritical fluid behavior at nanoscale interfaces: Implications for CO₂sequestration in geologic formations. Philosophical Magazine, 2010, 90, 2339-2363.	0.7	111
42	Structural Origins of Potential Dependent Hysteresis at the Electrified Graphene/Ionic Liquid Interface. Journal of Physical Chemistry C, 2014, 118, 569-574.	1.5	111
43	Enhancing graphene capacitance by nitrogen: effects of doping configuration and concentration. Physical Chemistry Chemical Physics, 2016, 18, 4668-4674.	1.3	110
44	Molecular Dynamics Study of the Structure and Thermophysical Properties of Model sI Clathrate Hydrates. Journal of Physical Chemistry B, 2002, 106, 442-451.	1.2	109
45	Generation of percolation cluster perimeters by a random walk. Journal of Physics A, 1984, 17, 3009-3017.	1.6	107
46	The oscillatory damped behaviour of incommensurate double-walled carbon nanotubes. Nanotechnology, 2005, 16, 186-198.	1.3	106
47	Hydration structure of water confined between mica surfaces. Journal of Chemical Physics, 2006, 124, 074711.	1.2	105
48	Multiple time step nonequilibrium molecular dynamics simulation of the rheological properties of liquid nâ€decane. Journal of Chemical Physics, 1996, 104, 255-262.	1.2	104
49	Molecular Simulation of a Dichain Surfactant/Water/Carbon Dioxide System. 1. Structural Properties of Aggregates. Langmuir, 2001, 17, 1773-1783.	1.6	101
50	Determination of the Gibbs Free Energy of Gas Replacement in SI Clathrate Hydrates by Molecular Simulation. Journal of Physical Chemistry A, 2002, 106, 7982-7987.	1.1	101
51	Mathematical modeling of cancer: The future of prognosis and treatment. Clinica Chimica Acta, 2005, 357, 173-179.	0.5	96
52	Phase Transformations during Sintering of Titania Nanoparticles. ACS Nano, 2008, 2, 1620-1624.	7.3	96
53	Intermolecular potentials and vaporâ€“liquid phase equilibria of perfluorinated alkanes. Fluid Phase Equilibria, 1998, 146, 51-61.	1.4	92
54	Simulated water adsorption isotherms in carbon nanopores. Molecular Physics, 2004, 102, 243-251.	0.8	91

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55	SHARP REGULARITY COEFFICIENT ESTIMATES FOR COMPLEX-VALUED ACOUSTIC AND ELASTIC HELMHOLTZ EQUATIONS. Mathematical Models and Methods in Applied Sciences, 2006, 16, 139-160.	1.7	90
56	A molecular dynamics study of a short-chain polyethylene melt.. Journal of Non-Newtonian Fluid Mechanics, 2000, 93, 83-99.	1.0	89
57	Self-Assembly of Reverse Micelles in Water/Surfactant/Carbon Dioxide Systems by Molecular Simulation. Langmuir, 1999, 15, 5188-5192.	1.6	88
58	Surface Protonation at the Rutile (110) Interface: Explicit Incorporation of Solvation Structure within the Refined MUSIC Model Framework. Langmuir, 2008, 24, 12331-12339.	1.6	88
59	Cellular Dynamics simulations of bacterial chemotaxis. Chemical Engineering Science, 1993, 48, 687-699.	1.9	87
60	Recent developments in non-Newtonian molecular dynamics. Physics Reports, 1998, 305, 1-92.	10.3	87
61	Rheology of lubricant basestocks: A molecular dynamics study of C30 isomers. Journal of Chemical Physics, 2000, 113, 8833-8840.	1.2	84
62	Molecular Dynamics Study of Water Adsorption on TiO2Nanoparticles. Journal of Physical Chemistry C, 2007, 111, 6920-6926.	1.5	84
63	Precision and accuracy of staged free-energy perturbation methods for computing the chemical potential by molecular simulation. Fluid Phase Equilibria, 1998, 150-151, 41-49.	1.4	80
64	Molecular simulation study of solvation structure in supercritical aqueous solutions. Chemical Engineering Science, 1994, 49, 2735-2748.	1.9	79
65	Dynamics of Hydration Water on Rutile Studied by Backscattering Neutron Spectroscopy and Molecular Dynamics Simulation. Journal of Physical Chemistry C, 2008, 112, 12334-12341.	1.5	79
66	An Off-Lattice Hybrid Discrete-Continuum Model of Tumor Growth and Invasion. Biophysical Journal, 2010, 98, 37-47.	0.2	79
67	Shear behavior of squalane and tetracosane under extreme confinement. I. Model, simulation method, and interfacial slip. Journal of Chemical Physics, 1997, 107, 10316-10326.	1.2	78
68	Electric Double Layer at the Rutile (110) Surface. 3. Inhomogeneous Viscosity and Diffusivity Measurement by Computer Simulations. Journal of Physical Chemistry C, 2007, 111, 3071-3079.	1.5	78
69	Simulated water adsorption in chemically heterogeneous carbon nanotubes. Journal of Chemical Physics, 2006, 124, 074710.	1.2	76
70	Solvation in supercritical water. Fluid Phase Equilibria, 1992, 71, 1-16.	1.4	74
71	Critical behavior of the Yukawa fluid in the mean spherical approximation. Journal of Chemical Physics, 1983, 78, 1917-1923.	1.2	73
72	Random walk calculations for bacterial migration in porous media. Biophysical Journal, 1995, 68, 800-806.	0.2	73

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73	Investigating the Quartz (101Ì…0)/Water Interface using Classical and Ab Initio Molecular Dynamics. Langmuir, 2011, 27, 8700-8709.	1.6	72
74	Statistical mechanical models of chemical reactions. Molecular Physics, 1985, 55, 33-48.	0.8	69
75	Scheduling of serial multiproduct batch processes via simulated annealing. Computers and Chemical Engineering, 1990, 14, 1351-1362.	2.0	69
76	Molecular Insights into Carbon Nanotube Supercapacitors: Capacitance Independent of Voltage and Temperature. Journal of Physical Chemistry C, 2013, 117, 9178-9186.	1.5	69
77	Interfacial ionic â€˜liquidsâ€™: connecting static and dynamic structures. Journal of Physics Condensed Matter, 2015, 27, 032101.	0.7	67
78	Distinctive Nanoscale Organization of Dicationic versus Monocationic Ionic Liquids. Journal of Physical Chemistry C, 2013, 117, 18251-18257.	1.5	66
79	Exact asymptotic form of the site-site direct correlation function for rigid polar molecules. Molecular Physics, 1981, 44, 529-531.	0.8	65
80	Algorithmic efficiency of simulated annealing for heat exchanger network design. Computers and Chemical Engineering, 1990, 14, 1039-1050.	2.0	65
81	On the Yukawa closure of the Ornstein-Zernike equation. Molecular Physics, 1979, 38, 997-1001.	0.8	64
82	Simple transferable intermolecular potential for the molecular simulation of water over wide ranges of state conditions. Fluid Phase Equilibria, 1998, 150-151, 73-81.	1.4	64
83	Examining the rheology of 9-octylheptadecane to giga-pascal pressures. Journal of Chemical Physics, 2001, 114, 1887-1891.	1.2	64
84	Evaluation of Force Fields for Molecular Simulation of Polyhedral Oligomeric Silsesquioxanes. Journal of Physical Chemistry B, 2006, 110, 2502-2510.	1.2	64
85	Engineering the Interlayer Spacing by Preâ€Intercalation for High Performance Supercapacitor MXene Electrodes in Room Temperature Ionic Liquid. Advanced Functional Materials, 2021, 31, 2104007.	7.8	64
86	Percus-Yevick theory of correlation functions and nucleation effects in the sticky hard-sphere model. Molecular Physics, 1976, 31, 535-548.	0.8	63
87	Molecular dynamics study of the nano-rheology ofn-dodecane confined between planar surfaces. Journal of Chemical Physics, 2003, 118, 8941-8944.	1.2	63
88	Electric Double Layer at Metal Oxide Surfaces:Â Static Properties of the Cassiteriteâ^'Water Interface. Langmuir, 2007, 23, 4925-4937.	1.6	63
89	Mean spherical approximation for a model liquid metal potential. Molecular Physics, 1981, 43, 1267-1291.	0.8	62
90	Molecular-Based Modeling of Water and Aqueous Solutions at Supercritical Conditions. Advances in Chemical Physics, 2007, , 115-205.	0.3	61

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91	Suppression of the dynamic transition in surface water at low hydration levels: A study of water on rutile. Physical Review E, 2009, 79, 051504.	0.8	61
92	Nonequilibrium molecular dynamics calculation of selfâ€diffusion in a nonâ€Newtonian fluid subject to a Couette strain field. Journal of Chemical Physics, 1991, 94, 2149-2158.	1.2	60
93	Vapor-Liquid Phase Coexistence of Alkaneâ^'Carbon Dioxide and Perfluoroalkaneâ^'Carbon Dioxide Mixtures. Journal of Physical Chemistry B, 1999, 103, 4485-4491.	1.2	60
94	Dynamic and Structural Properties of Room-Temperature Ionic Liquids near Silica and Carbon Surfaces. Langmuir, 2013, 29, 9744-9749.	1.6	59
95	A model for association in electrolytes. Analytic solution of the hypernettedâ€chain/mean spherical approximation. Journal of Chemical Physics, 1985, 83, 317-325.	1.2	58
96	Scalable Screening of Soft Matter: A Case Study of Mixtures of Ionic Liquids and Organic Solvents. Journal of Physical Chemistry B, 2019, 123, 1340-1347.	1.2	58
97	Experimental measurement of vapor-liquid equilibrium in alcohol/water/salt systems. Journal of Chemical & Engineering Data, 1990, 35, 395-404.	1.0	57
98	Thermodynamic and Transport Properties of Polyhedral Oligomeric Sislesquioxanes in Poly(dimethylsiloxane). Journal of Physical Chemistry B, 2005, 109, 14300-14307.	1.2	57
99	Molecular dynamics simulations of stretched gold nanowires: The relative utility of different semiempirical potentials. Journal of Chemical Physics, 2007, 126, 144707.	1.2	57
100	Fundamental aspects of electric double layer force-distance measurements at liquid-solid interfaces using atomic force microscopy. Scientific Reports, 2016, 6, 32389.	1.6	57
101	Liquidâ€"gas transition for hard spheres with attractive Yukawa tail interactions. Chemical Physics, 1979, 42, 241-247.	0.9	56
102	Ejection of atoms upon self-trapping of an atomic exciton in solid argon. Physical Review B, 1989, 39, 9580-9583.	1.1	56
103	Vaporâ€"liquid equilibrium simulations of the SCPDP model of water. Chemical Physics Letters, 2002, 357, 189-194.	1.2	56
104	In Situ Electrochemical Dilatometry of Onion-Like Carbon and Carbon Black. Journal of the Electrochemical Society, 2012, 159, A1897-A1903.	1.3	56
105	Densification of Ionic Liquid Molecules within a Hierarchical Nanoporous Carbon Structure Revealed by Small-Angle Scattering and Molecular Dynamics Simulation. Chemistry of Materials, 2014, 26, 1144-1153.	3.2	55
106	Pre-Sodiated Ti₃C₂T_x MXene Structure and Behavior as Electrode for Sodium-Ion Capacitors. ACS Nano, 2021, 15, 2994-3003.	7.3	54
107	Perturbation Expansion of Alt's Cell Balance Equations Reduces to Segel's One-Dimensional Equations for Shallow Chemoattractant Gradients. SIAM Journal on Applied Mathematics, 1998, 59, 35-57.	0.8	53
108	Steady state simulation of planar elongation flow by nonequilibrium molecular dynamics. Journal of Chemical Physics, 1999, 110, 42-45.	1.2	53

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109	Layering Behavior and Axial Phase Equilibria of Pure Water and Water + Carbon Dioxide Inside Single Wall Carbon Nanotubes. Nano Letters, 2002, 2, 1427-1431.	4.5	53
110	Comment on â€˜Near critical phase behaviour of dilute mixturesâ€™. Molecular Physics, 1995, 84, 41-48.	0.8	52
111	Molecular Simulation Study of Tetraalkylammonium Halides. 1. Solvation Structure and Hydrogen Bonding in Aqueous Solutions. Journal of Physical Chemistry B, 1997, 101, 3818-3826.	1.2	52
112	Molecular dynamics simulation of the limiting conductance of NaCl in supercritical water. Chemical Physics Letters, 1998, 293, 289-294.	1.2	51
113	Solvation in high-temperature electrolyte solutions. II. Some formal results. Journal of Chemical Physics, 1999, 110, 1075-1086.	1.2	51
114	Calculation of Viscous EHL Traction for Squalane Using Molecular Simulation and Rheometry. Tribology Letters, 2002, 13, 251-254.	1.2	51
115	Molecular dynamics simulation of limiting conductances for LiCl, NaBr, and CsBr in supercritical water. Journal of Chemical Physics, 2000, 112, 864-869.	1.2	50
116	Solution of the Ornsteinâ€“Zernike equation in the vicinity of the critical point of a simple fluid. Journal of Chemical Physics, 1985, 82, 4303-4311.	1.2	49
117	Anomalies in the Solubility of Alkanes in Near-Critical Water. Journal of Physical Chemistry B, 2003, 107, 12307-12314.	1.2	49
118	Sintering of titanium dioxide nanoparticles: a comparison between molecular dynamics and phenomenological modeling. Journal of Nanoparticle Research, 2008, 10, 1169-1182.	0.8	49
119	Temperature and density effects on the high temperature ionic speciation in dilute Na+/Clâ¯aqueous solutions. Journal of Chemical Physics, 1996, 105, 9248-9257.	1.2	48
120	Effect of the Range of Interactions on the Properties of Fluids. Phase Equilibria in Pure Carbon Dioxide, Acetone, Methanol, and Water. Journal of Physical Chemistry B, 2002, 106, 7537-7546.	1.2	48
121	Dielectric constant of dipolar hard sphere mixtures. Journal of Chemical Physics, 1986, 85, 6658-6667.	1.2	47
122	Shear behavior of squalane and tetracosane under extreme confinement. III. Effect of confinement on viscosity. Journal of Chemical Physics, 1997, 107, 10335-10343.	1.2	47
123	Comment on â€œStructure and dynamics of liquid water on rutile TiO2(110)â€• Physical Review B, 2012, 85, .	1.1	46
124	The Electrical Double Layer of Dicationic Ionic Liquids at Onion-like Carbon Surface. Journal of Physical Chemistry C, 2014, 118, 3901-3909.	1.5	46
125	Gibbs ensemble simulation of phase equilibrium in the hard core two-Yukawa fluid model for the Lennard-Jones fluid. Molecular Physics, 1989, 68, 629-635.	0.8	45
126	Solvation in high-temperature electrolyte solutions. I. Hydration shell behavior from molecular simulation. Journal of Chemical Physics, 1999, 110, 1064-1074.	1.2	45

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127	Solvent Polarity Governs Ion Interactions and Transport in a Solvated Room-Temperature Ionic Liquid. Journal of Physical Chemistry Letters, 2017, 8, 167-171.	2.1	45
128	Simulated Water Adsorption Isotherms in Hydrophilic and Hydrophobic Cylindrical Nanopores. Adsorption, 2005, 11, 397-401.	1.4	43
129	Aqua Ionsâ€“Graphene Interfacial and Confinement Behavior: Insights from Isobaricâ€“Isothermal Molecular Dynamics. Journal of Physical Chemistry A, 2011, 115, 5918-5927.	1.1	43
130	A DFT study of water adsorption on rutile TiO2 (110) surface: The effects of surface steps. Journal of Chemical Physics, 2016, 145, 044702.	1.2	43
131	Computer simulation of dipolar fluids. Dependence of the dielectric constant on system size: A comparative study of Ewald sum and reaction field approaches. Journal of Chemical Physics, 1986, 85, 1502-1504.	1.2	42
132	Shear behavior of squalane and tetracosane under extreme confinement. II. Confined film structure. Journal of Chemical Physics, 1997, 107, 10327-10334.	1.2	42
133	Configurational bias Gibbs ensemble Monte Carlo simulation of vapor-liquid equilibria of linear and short-branched alkanes. Fluid Phase Equilibria, 1997, 141, 45-61.	1.4	42
134	Solvation effect on kinetic rate constant of reactions in supercritical solvents. AICHE Journal, 1998, 44, 667-680.	1.8	42
135	Polarizable contributions to the surface tension of liquid water. Journal of Chemical Physics, 2006, 125, 094712.	1.2	42
136	Self-Assembly of 1,4-Benzenedithiolate/Tetrahydrofuran on a Gold Surface:Â A Monte Carlo Simulation Study. Langmuir, 2006, 22, 4116-4124.	1.6	42
137	Molecular Dynamics Simulation Study of the Capacitive Performance of a Binary Mixture of Ionic Liquids near an Onion-like Carbon Electrode. Journal of Physical Chemistry Letters, 2012, 3, 2465-2469.	2.1	42
138	Shear viscosity of a simple fluid over a wide range of strain rates. Molecular Physics, 2002, 100, 2735-2738.	0.8	41
139	Computational chemistry for molecular electronics. Computational Materials Science, 2003, 28, 321-341.	1.4	41
140	Phase Transitions of Water in Graphite and Mica Pores. Journal of Physical Chemistry C, 2011, 115, 12448-12457.	1.5	41
141	Statistical mechanical models of chemical reactions. Molecular Physics, 1987, 60, 1315-1342.	0.8	40
142	Nonequilibrium Molecular Dynamics Simulation of the Rheology of Linear and Branched Alkanes. International Journal of Thermophysics, 1998, 19, 449-459.	1.0	40
143	The structure of water from 25Â°C to 457Â°C: comparison between neutron scattering and molecular simulation. Chemical Physics, 2000, 258, 109-120.	0.9	40
144	Modeling the Interaction between Integrin-Binding Peptide (RGD) and Rutile Surface: The Effect of Cation Mediation on Asp Adsorption. Langmuir, 2012, 28, 2799-2811.	1.6	40

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145	Effect of cation on diffusion coefficient of ionic liquids at onion-like carbon electrodes. Journal of Physics Condensed Matter, 2014, 26, 284104.	0.7	40
146	Influence of Surface Oxidation on Ion Dynamics and Capacitance in Porous and Nonporous Carbon Electrodes. Journal of Physical Chemistry C, 2016, 120, 8730-8741.	1.5	40
147	The dielectric constant of polar hard dumb-bells. Molecular Physics, 1982, 45, 1099-1112.	0.8	39
148	On the Relationship Between Cell Balance Equations for Chemotactic Cell Populations. SIAM Journal on Applied Mathematics, 1992, 52, 1426-1441.	0.8	39
149	Molecular Simulation of a Dichain Surfactant/Water/Carbon Dioxide System. 2. Self-Assembly and Aggregation Dynamics. Langmuir, 2001, 17, 1784-1792.	1.6	39
150	Molecular simulations of stretching gold nanowires in solvents. Nanotechnology, 2007, 18, 424007.	1.3	39
151	Phase transitions in nanoconfined fluids: The evidence from simulation and theory. AICHE Journal, 2010, 56, 842-848.	1.8	39
152	Strainâ€Based In Situ Study of Anion and Cation Insertion into Porous Carbon Electrodes with Different Pore Sizes. Advanced Energy Materials, 2014, 4, 1300683.	10.2	39
153	Molecular Dynamics Study of Alkylsilane Monolayers on Realistic Amorphous Silica Surfaces. Langmuir, 2015, 31, 3086-3093.	1.6	39
154	Auxiliary sites in the RISM approximation for molecular fluids. Journal of Physics A, 1981, 14, 1483-1512.	1.6	38
155	Analytic solution of the molecular Ornsteinâ€“Zernike equation for nonspherical molecules. Spheres with anisotropic surface adhesion. Journal of Chemical Physics, 1986, 84, 1833-1842.	1.2	38
156	Computer Simulation of the Dielectric Properties of Liquid Water. Molecular Simulation, 1989, 2, 89-104.	0.9	38
157	Molecular Dynamics Simulation of Reverse Micelles in Supercritical Carbon Dioxide. Industrial & Engineering Chemistry Research, 2000, 39, 4543-4554.	1.8	38
158	Effective Interactions between Polyhedral Oligomeric Sislesquioxanes Dissolved in Normal Hexadecane from Molecular Simulation. Macromolecules, 2005, 38, 8950-8959.	2.2	38
159	Shear dynamics of hydration layers. Journal of Chemical Physics, 2006, 125, 104701.	1.2	38
160	Coarse-grained force field for simulating polymer-tethered silsesquioxane self-assembly in solution. Journal of Chemical Physics, 2007, 127, 114102.	1.2	38
161	Atomistic simulations of highly conductive molecular transport junctions under realistic conditions. Nanoscale, 2013, 5, 3654.	2.8	38
162	Classical dynamics description of low energy cascades in solids: Atomic ejection from solid argon. Surface Science, 1988, 207, 186-206.	0.8	37

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163	Interplay between Molecular Simulation and Neutron Scattering in Developing New Insights into the Structure of Waterâ€. Industrial & Engineering Chemistry Research, 1998, 37, 3021-3025.	1.8	37
164	Molecular simulation of the temperature- and density-dependence of ionic hydration in aqueous SrCl2 solutions using rigid and flexible water models. Journal of Chemical Physics, 1999, 111, 5141-5149.	1.2	37
165	Characterizing the viscosityâ€“temperature dependence of lubricants by molecular simulation. Fluid Phase Equilibria, 2001, 183-184, 363-370.	1.4	37
166	Organic-inorganic telechelic molecules: Solution properties from simulations. Journal of Chemical Physics, 2006, 125, 104904.	1.2	37
167	Human Mammary Epithelial Cells Exhibit a Bimodal Correlated Random Walk Pattern. PLoS ONE, 2010, 5, e9636.	1.1	37
168	Non-equilibrium molecular dynamics simulation of dense fluid methane. Chemical Physics Letters, 1986, 129, 92-98.	1.2	36
169	Molecular dynamics simulation of the rheological and dynamical properties of a model alkane fluid under confinement. Journal of Chemical Physics, 1999, 111, 1273-1280.	1.2	36
170	H3O+/Clâ¯ ion-pair formation in high-temperature aqueous solutions. Journal of Chemical Physics, 2000, 113, 8093-8100.	1.2	36
171	Predicting the Newtonian viscosity of complex fluids from high strain rate molecular simulations. Journal of Chemical Physics, 2002, 116, 3339-3342.	1.2	36
172	Hydrogen bonding and induced dipole moments in water: Predictions from the Gaussian charge polarizable model and Car-Parrinello molecular dynamics. Journal of Chemical Physics, 2006, 125, 144519.	1.2	36
173	Adsorption of Arginineâ€“Glycineâ€“Aspartate Tripeptide onto Negatively Charged Rutile (110) Mediated by Cations: The Effect of Surface Hydroxylation. ACS Applied Materials & Interfaces, 2013, 5, 2567-2579.	4.0	36
174	A Hierarchical, Component Based Approach to Screening Properties of Soft Matter. Molecular Modeling and Simulation, 2016, , 79-92.	0.2	36
175	Computational insight into the capacitive performance of graphene edge planes. Carbon, 2017, 116, 278-285.	5.4	36
176	Ionic liquid structure, dynamics, and electrosorption in carbon electrodes with bimodal pores and heterogeneous surfaces. Carbon, 2018, 129, 104-118.	5.4	36
177	Nonequilibrium molecular dynamics study of shear and shearâ€free flows in simple fluids. Journal of Chemical Physics, 1995, 103, 10217-10225.	1.2	35
178	Residence time calculation for chemotactic bacteria within porous media. Biophysical Journal, 1997, 73, 2930-2936.	0.2	35
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