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	Beyond Simple Dilution: Superior Conductivities from Cosolvation of Acetonitrile/LiTFSI Concentrated Solution with Acetone. Journal of Physical Chemistry C, 2022, 126, 2788-2796.	1.5	6
2	High-throughput screening of tribological properties of monolayer films using molecular dynamics and machine learning. Journal of Chemical Physics, 2022, 156, 154902.	1.2	5
3	Investigation of Multilayered Structures of Ionic Liquids on Graphite and Platinum Using Atomic Force Microscopy and Molecular Simulations. Langmuir, 2022, 38, 4036-4047.	1.6	5
4	Continuous transition from double-layer to Faradaic charge storage in confined electrolytes. Nature Energy, 2022, 7, 222-228.	19.8	130
5	Direct Correlation of the Salt-Reduced Diffusivities of Organic Solvents with the Solventâ€™s Mole Fraction. Journal of Physical Chemistry Letters, 2022, 13, 2845-2850.	2.1	2
6	Empty liquid state and re-entrant phase behavior of the patchy colloids confined in porous media. Journal of Chemical Physics, 2022, 156, 161102.	1.2	4
7	NMR and Theoretical Study of In-Pore Diffusivity of Ionic Liquidâ€“Solvent Mixtures. Journal of Physical Chemistry B, 2022, 126, 4889-4898.	1.2	3
8	Controlling the Ion Transport Number in Solvent-in-Salt Solutions. Journal of Physical Chemistry B, 2022, 126, 4572-4583.	1.2	5
9	Borasilylenes in Focus: Topological Effects of Nitrogen Atoms by DFT. Silicon, 2021, 13, 3377-3383.	1.8	6
10	Engineering for Inclusion: Empowering Individuals with Physical and Neurological Differences through Engineering Invention, Research, and Development. Engineering, 2021, 7, 141-143.	3.2	0
11	Integral equation theory for mixtures of spherical and patchy colloids. 2. Numerical results. Soft Matter, 2021, 17, 3513-3519.	1.2	5
12	A tribute to Keith E. Gubbins. AICHE Journal, 2021, 67, e17187.	1.8	0
13	Keith E. Gubbins: A retrospective. AICHE Journal, 2021, 67, e17191.	1.8	0
14	Openâ€source molecular modeling software in chemical engineering focusing on the Molecular Simulation Design Framework. AICHE Journal, 2021, 67, e17206.	1.8	16
15	MoSDeF Cassandra: A complete Python interface for the Cassandra Monte Carlo software. Journal of Computational Chemistry, 2021, 42, 1321-1331.	1.5	4
16	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
17	Engineering the Interlayer Spacing by Preâ€Intercalation for High Performance Supercapacitor MXene Electrodes in Room Temperature Ionic Liquid (Adv. Funct. Mater. 33/2021). Advanced Functional Materials, 2021, 31, 2170246.	7.8	2
18	Investigating the Accuracy of Water Models through the Van Hove Correlation Function. Journal of Chemical Theory and Computation, 2021, 17, 5992-6005.	2.3	9

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19	A mathematical model for Escherichia coli chemotaxis to competing stimuli. Biotechnology and Bioengineering, 2021, 118, 4678-4686.	1.7	4
20	Pre-Sodiated Ti₃C₂T_x MXene Structure and Behavior as Electrode for Sodium-Ion Capacitors. ACS Nano, 2021, 15, 2994-3003.	7.3	54
21	In situ investigation of water on MXene interfaces. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	24
22	Addition of Chloroform in a Solvent-in-Salt Electrolyte: Outcomes in the Microscopic Dynamics in Bulk and Confinement. Journal of Physical Chemistry C, 2020, 124, 22366-22375.	1.5	7
23	Diffusivity and Structure of Room Temperature Ionic Liquid in Various Organic Solvents. Journal of Physical Chemistry B, 2020, 124, 9931-9937.	1.2	18
24	Integral equation theory for a mixture of spherical and patchy colloids: analytical description. Soft Matter, 2020, 16, 3456-3465.	1.2	8
25	Molecular investigations of tripeptide adsorption onto TiO2 surfaces: Synergetic effects of surface nanostructure, hydroxylation and bioactive ions. Applied Surface Science, 2020, 512, 145713.	3.1	8
26	MoSDeF, a Python Framework Enabling Large-Scale Computational Screening of Soft Matter: Application to Chemistry-Property Relationships in Lubricating Monolayer Films. Journal of Chemical Theory and Computation, 2020, 16, 1779-1793.	2.3	22
27	Critical Role of Anionâ€“Solvent Interactions for Dynamics of Solvent-in-Salt Solutions. Journal of Physical Chemistry C, 2020, 124, 8457-8466.	1.5	32
28	Towards molecular simulations that are transparent, reproducible, usable by others, and extensible (TRUE). Molecular Physics, 2020, 118, e1742938.	0.8	22
29	Formalizing atom-typing and the dissemination of force fields with foyer. Computational Materials Science, 2019, 167, 215-227.	1.4	29
30	Microscopic Dynamics in an Ionic Liquid Augmented with Organic Solvents. Journal of Physical Chemistry C, 2019, 123, 19354-19361.	1.5	8
31	Computational Modeling of Particle Hydrodynamics and Charging Process for the Flowable Electrodes of Carbon Slurry. Journal of the Electrochemical Society, 2019, 166, A2643-A2653.	1.3	10
32	Effects of Solvent Concentration on the Performance of Ionic-Liquid/Carbon Supercapacitors. ACS Applied Materials & Interfaces, 2019, 11, 42680-42689.	4.0	25
33	Ion Pairing Controls Physical Properties of Ionic Liquid-Solvent Mixtures. Journal of Physical Chemistry B, 2019, 123, 9944-9955.	1.2	25
34	Identifying Waterâ€“Anion Correlated Motion in Aqueous Solutions through Van Hove Functions. Journal of Physical Chemistry Letters, 2019, 10, 7119-7125.	2.1	13
35	Molecular Investigation of Oxidized Graphene: Anatomy of the Double-Layer Structure and Ion Dynamics. Journal of Physical Chemistry C, 2019, 123, 12583-12591.	1.5	15
36	Open-source molecular modeling software in chemical engineering. Current Opinion in Chemical Engineering, 2019, 23, 99-105.	3.8	6

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37	Investigation of the Impact of Cross-Polymerization on the Structural and Frictional Properties of Alkylsilane Monolayers Using Molecular Simulation. Nanomaterials, 2019, 9, 639.	1.9	11
38	A Transferable, Multi-Resolution Coarse-Grained Model for Amorphous Silica Nanoparticles. Journal of Chemical Theory and Computation, 2019, 15, 3260-3271.	2.3	8
39	Nucleophilicity of cyclic conjugated silylenes using DFT method. Journal of Physical Organic Chemistry, 2019, 32, e3956.	0.9	13
40	Novel triplet germylenes in focus: normal vs. abnormal triplet exocyclic tetrazol-5-vinylidene germylenes at DFT. Journal of Molecular Modeling, 2019, 25, 371.	0.8	1
41	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
42	Gallic acid-functionalized magnetic nanoparticles: a convenient and green approach for synthesis of Î±-aminonitriles under solvent-free conditions. Research on Chemical Intermediates, 2019, 45, 303-314.	1.3	3
43	Phase Equilibria of Polydisperse Square-Well Chain Fluid Confined in Random Porous Media: TPT of Wertheim and Scaled Particle Theory. Journal of Physical Chemistry B, 2018, 122, 5458-5465.	1.2	6
44	Î²-Enaminones over recyclable nano-CoFe2O4: a highly efficient solvent-free green protocol. Research on Chemical Intermediates, 2018, 44, 5787-5799.	1.3	10
45	Ionic liquid structure, dynamics, and electrosorption in carbon electrodes with bimodal pores and heterogeneous surfaces. Carbon, 2018, 129, 104-118.	5.4	36
46	Humidity Exposure Enhances Microscopic Mobility in a Room-Temperature Ionic Liquid in MXene. Journal of Physical Chemistry C, 2018, 122, 27561-27566.	1.5	20
47	Mobilities of polydisperse hard spheres near a no-slip wall. Computers and Fluids, 2018, 176, 40-50.	1.3	5
48	Synthesis of quinazolines over recyclable Fe₃O₄@SiO₂â€PrNH₂â€Fe³⁺ nanoparticles: A green, efficient, and solventâ€free protocol. Applied Organometallic Chemistry, 2018, 32, e4573.	1.7	18
49	Electrolyte cation length influences electrosorption and dynamics in porous carbon supercapacitors. Electrochimica Acta, 2018, 283, 882-893.	2.6	25
50	Molecular Investigation of the Initial Nucleation of Calcium Phosphate on TiO₂ Substrate: The Effects of Surface Nanotopographies. Crystal Growth and Design, 2018, 18, 3283-3290.	1.4	10
51	Computational insight into the capacitive performance of graphene edge planes. Carbon, 2017, 116, 278-285.	5.4	36
52	Melting upon cooling and freezing upon heating: fluidâ€“solid phase diagram for Åvejkâ€“HaÅ¡ek model of dimerizing hard spheres. Soft Matter, 2017, 13, 1156-1160.	1.2	4
53	Computational Insights into Materials and Interfaces for Capacitive Energy Storage. Advanced Science, 2017, 4, 1700059.	5.6	176
54	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

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55	Investigating Alkylsilane Monolayer Tribology at a Single-Asperity Contact with Molecular Dynamics Simulation. Langmuir, 2017, 33, 11270-11280.	1.6	23
56	An Atomistic Carbide-Derived Carbon Model Generated Using ReaxFF-Based Quenched Molecular Dynamics. Journal of Carbon Research, 2017, 3, 32.	1.4	13
57	Influence of humidity on performance and microscopic dynamics of an ionic liquid in supercapacitor. Physical Review Materials, 2017, 1, .	0.9	15
58	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
59	Relationship between pore size and reversible and irreversible immobilization of ionic liquid electrolytes in porous carbon under applied electric potential. Applied Physics Letters, 2016, 109, .	1.5	23
60	Molecular simulation study of dynamical properties of room temperature ionic liquids with carbon pieces. Science China Chemistry, 2016, 59, 594-600.	4.2	2
61	Molecular modeling of fibronectin adsorption on topographically nanostructured rutile (110) surfaces. Applied Surface Science, 2016, 384, 36-44.	3.1	14
62	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
63	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
64	A Hierarchical, Component Based Approach to Screening Properties of Soft Matter. Molecular Modeling and Simulation, 2016, , 79-92.	0.2	36
65	Molecular mechanics of the cooperative adsorption of a Pro-Hyp-Gly tripeptide on a hydroxylated rutile TiO₂(110) surface mediated by calcium ions. Physical Chemistry Chemical Physics, 2016, 18, 19757-19764.	1.3	11
66	Enhancing graphene capacitance by nitrogen: effects of doping configuration and concentration. Physical Chemistry Chemical Physics, 2016, 18, 4668-4674.	1.3	110
67	Influence of Surface Morphology on the Shear-Induced Wear of Alkylsilane Monolayers: Molecular Dynamics Study. Langmuir, 2016, 32, 2348-2359.	1.6	13
68	Examining the aggregation behavior of polymer grafted nanoparticles using molecular simulation and theory. Journal of Chemical Physics, 2015, 143, 054904.	1.2	10
69	Examination of the phase transition behavior of nano-confined fluids by statistical temperature molecular dynamics. Journal of Chemical Physics, 2015, 143, 054504.	1.2	7
70	Microstructure of room temperature ionic liquids at stepped graphite electrodes. AICHE Journal, 2015, 61, 3022-3028.	1.8	32
71	A tribute to John M. Prausnitz. AICHE Journal, 2015, 61, 2674-2674.	1.8	0
72	A Computational Study of Dicationic Ionic Liquids/CO₂ Interfaces. Langmuir, 2015, 31, 2447-2454.	1.6	23

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73	Prediction of n-Alkane Adsorption on Activated Carbon Using the SAFTâ€“FMTâ€“DFT Approach. Journal of Physical Chemistry C, 2015, 119, 1457-1463.	1.5	14
74	Thickness-dependent structural arrangement in nano-confined imidazolium-based ionic liquid films. Physical Chemistry Chemical Physics, 2015, 17, 4152-4159.	1.3	16
75	Interfacial ionic â€˜liquidsâ€™: connecting static and dynamic structures. Journal of Physics Condensed Matter, 2015, 27, 032101.	0.7	67
76	Topological defects in electric double layers of ionic liquids at carbon interfaces. Nano Energy, 2015, 15, 737-745.	8.2	35
77	Compounding effects of fluid confinement and surface strain on the wetâ€“dry transition, thermodynamic response, and dynamics of waterâ€“graphene systems. Molecular Physics, 2015, 113, 1033-1042.	0.8	1
78	Molecular Dynamics Study of Alkylsilane Monolayers on Realistic Amorphous Silica Surfaces. Langmuir, 2015, 31, 3086-3093.	1.6	39
79	Tunable transition from hydration to monomer-supported lubrication in zwitterionic monolayers revealed by molecular dynamics simulation. Soft Matter, 2015, 11, 3340-3346.	1.2	22
80	Modeling of Supercapacitors. , 2015, , 2282-2289.		0
81	Simulating Phase Equilibria using Wang-Landau-Transition Matrix Monte Carlo. Journal of Physics: Conference Series, 2014, 487, 012002.	0.3	11
82	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
83	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
84	Toward understanding the structural heterogeneity and ion pair stability in dicationic ionic liquids. Soft Matter, 2014, 10, 9193-9200.	1.2	30
85	Interfaces of dicationic ionic liquids and graphene: a molecular dynamics simulation study. Journal of Physics Condensed Matter, 2014, 26, 284106.	0.7	32
86	Integrated Experimental and Computational Studies of Energy-relevant Interfaces. Physics Procedia, 2014, 53, 32-38.	1.2	0
87	The influence of a hierarchical porous carbon network on the coherent dynamics of a nanoconfined room temperature ionic liquid: A neutron spin echo and atomistic simulation investigation. Carbon, 2014, 78, 415-427.	5.4	24
88	Surface Strain Effects on the Waterâ€“Graphene Interfacial and Confinement Behavior. Journal of Physical Chemistry C, 2014, 118, 19701-19711.	1.5	21
89	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
90	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

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91	Audibilization: Data Analysis by Ear. Journal of Chemical Theory and Computation, 2014, 10, 1387-1394.	2.3	1
92	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
93	Web- and Cloud-based Software Infrastructure for Materials Design. Procedia Computer Science, 2014, 29, 2034-2044.	1.2	7
94	A model-integrated computing approach to nanomaterials simulation. Theoretical Chemistry Accounts, 2013, 132, 1.	0.5	3
95	Human serum albumin interactions with C60 fullerene studied by spectroscopy, small-angle neutron scattering, and molecular dynamics simulations. Journal of Nanoparticle Research, 2013, 15, 1.	0.8	18
96	Examining the phase transition behavior of amphiphilic lipids in solution using statistical temperature molecular dynamics and replica-exchange Wang-Landau methods. Journal of Chemical Physics, 2013, 139, 054505.	1.2	18
97	Dynamic and Structural Properties of Room-Temperature Ionic Liquids near Silica and Carbon Surfaces. Langmuir, 2013, 29, 9744-9749.	1.6	59
98	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
99	Molecular Insights into Carbon Supercapacitors Based on Room-Temperature Ionic Liquids. Journal of Physical Chemistry Letters, 2013, 4, 3367-3376.	2.1	125
100	Surface Corrugation Effects on the Waterâ€“Graphene Interfacial and Confinement Behavior. Journal of Physical Chemistry C, 2013, 117, 23875-23886.	1.5	20
101	Adsorption of Chain Molecules in Slit-Shaped Pores: Development of a SAFT-FMT-DFT Approach. Journal of Physical Chemistry C, 2013, 117, 21337-21350.	1.5	15
102	Structural Origins of Conductance Fluctuations in Goldâ€“Thiolate Molecular Transport Junctions. Journal of Physical Chemistry Letters, 2013, 4, 887-891.	2.1	33
103	Probing the Statistical Validity of the Ductile-to-Brittle Transition in Metallic Nanowires Using GPU Computing. Journal of Chemical Theory and Computation, 2013, 9, 5558-5566.	2.3	8
104	Bias-Dependent Molecular-Level Structure of Electrical Double Layer in Ionic Liquid on Graphite. Nano Letters, 2013, 13, 5954-5960.	4.5	142
105	Atomistic simulations of highly conductive molecular transport junctions under realistic conditions. Nanoscale, 2013, 5, 3654.	2.8	38
106	Molecular Insights into Carbon Nanotube Supercapacitors: Capacitance Independent of Voltage and Temperature. Journal of Physical Chemistry C, 2013, 117, 9178-9186.	1.5	69
107	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
108	Distinctive Nanoscale Organization of Dicationic versus Monocationic Ionic Liquids. Journal of Physical Chemistry C, 2013, 117, 18251-18257.	1.5	66

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109	Modeling of Supercapacitors. , 2013, , 1-9.		0
110	In Situ Electrochemical Dilatometry of Onion-Like Carbon and Carbon Black. Journal of the Electrochemical Society, 2012, 159, A1897-A1903.	1.3	56
111	Comment on â€œStructure and dynamics of liquid water on rutile TiO2(110)â€• Physical Review B, 2012, 85, .	1.1	46
112	Confined fluid and the fluid-solid transition: Evidence from absolute free energy calculations. Physical Review B, 2012, 86, .	1.1	12
113	Nanoscale Perturbations of Room Temperature Ionic Liquid Structure at Charged and Uncharged Interfaces. ACS Nano, 2012, 6, 9818-9827.	7.3	151
114	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
115	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
116	Large-Scale Atomistic Simulations of Environmental Effects on the Formation and Properties of Molecular Junctions. ACS Nano, 2012, 6, 2779-2789.	7.3	26
117	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
118	Rotational and Translational Dynamics of N-Butyl-N-methylpiperidinium Trifluoromethanesulfonimide Ionic Liquids Studied by NMR and MD Simulations. Journal of Physical Chemistry C, 2012, 116, 20779-20786.	1.5	16
119	Fourier space approach to the classical density functional theory for multi-Yukawa and square-well fluids. Journal of Chemical Physics, 2012, 137, 104104.	1.2	12
120	Investigation of bone resorption within a cortical basic multicellular unit using a lattice-based computational model. Bone, 2012, 50, 378-389.	1.4	24
121	A Wang-Landau study of a lattice model for lipid bilayer self-assembly. Journal of Chemical Physics, 2012, 137, 144901.	1.2	4
122	Incorporating configurational-bias Monte Carlo into the Wang-Landau algorithm for continuous molecular systems. Journal of Chemical Physics, 2012, 137, 204105.	1.2	4
123	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
124	An improved thermodynamic perturbation theory for square-well m-point model of the patchy colloids. Journal of Chemical Physics, 2012, 137, 244910.	1.2	8
125	Effect of Electric Field on Water Confined in Graphite and Mica Pores. Journal of Physical Chemistry C, 2012, 116, 17594-17603.	1.5	25
126	Liquid-gas phase behavior of polydisperse dipolar hard-sphere fluid: Extended thermodynamic perturbation theory for central force associating potential. Condensed Matter Physics, 2012, 15, 23605.	0.3	2

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127	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
128	Modeling the Interaction between Integrin-Binding Peptide (RGD) and Rutile Surface: The Effect of Na⁺ on Peptide Adsorption. Journal of Physical Chemistry C, 2011, 115, 22375-22386.	1.5	21
129	The Influence of Molecular Adsorption on Elongating Gold Nanowires. Journal of Physical Chemistry C, 2011, 115, 18422-18433.	1.5	24
130	Fluctuations and Correlations in Physical and Biological Nanosystems: The Tale Is in the Tails. ACS Nano, 2011, 5, 2425-2432.	7.3	10
131	Comparison of Cation Adsorption by Isostructural Rutile and Cassiterite. Langmuir, 2011, 27, 4585-4593.	1.6	29
132	Role of Polytetrahedral Structures in the Elongation and Rupture of Gold Nanowires. ACS Nano, 2011, 5, 10065-10073.	7.3	18
133	Resummed thermodynamic perturbation theory for central force associating potential. Multi-patch models. Journal of Chemical Physics, 2011, 135, 014501.	1.2	30
134	Investigating the Quartz (101Ì…0)/Water Interface using Classical and Ab Initio Molecular Dynamics. Langmuir, 2011, 27, 8700-8709.	1.6	72
135	Phase Transitions of Water in Graphite and Mica Pores. Journal of Physical Chemistry C, 2011, 115, 12448-12457.	1.5	41
136	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
137	Supercapacitor Capacitance Exhibits Oscillatory Behavior as a Function of Nanopore Size. Journal of Physical Chemistry Letters, 2011, 2, 2859-2864.	2.1	316
138	Network Forming Fluids: Yukawa Square-Well m-Point Model. Journal of Statistical Physics, 2011, 145, 481-506.	0.5	14
139	Phase behavior of a simple model of ferrocolloidal fluid. Chemical Physics Letters, 2011, 503, 226-230.	1.2	0
140	Direct and quantitative comparison of pixelated density profiles with high-resolution X-ray reflectivityÂdata. Journal of Synchrotron Radiation, 2011, 18, 257-265.	1.0	18
141	Lamininâ€332 cleavage by matriptase alters motility parameters of prostate cancer cells. Prostate, 2011, 71, 184-196.	1.2	28
142	The importance of polarisability in the modelling of solubility: quantifying the effect of charged co-solutes on the solubility of small non-polar solutes. Molecular Simulation, 2011, 37, 299-309.	0.9	4
143	Chapter 4. Phase Transition under Confinement. RSC Theoretical and Computational Chemistry Series, 2011, , 82-108.	0.7	1
144	MULTISCALE SIMULATION. , 2011, , 185-198.		0

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145	Phase transitions in nanoconfined fluids: The evidence from simulation and theory. AIChE Journal, 2010, 56, 842-848.	1.8	39
146	Comparative studies on the structure and diffusion dynamics of aqueous and nonpolar liquid films under nanometers confinement. Modelling and Simulation in Materials Science and Engineering, 2010, 18, 034007.	0.8	7
147	Resummed thermodynamic perturbation theory for central force associating potential: One-patch model. Journal of Chemical Physics, 2010, 133, 044502.	1.2	34
148	An Off-Lattice Hybrid Discrete-Continuum Model of Tumor Growth and Invasion. Biophysical Journal, 2010, 98, 37-47.	0.2	79
149	Bimodal Analysis Reveals a General Scaling Law Governing Nondirected and Chemotactic Cell Motility. Biophysical Journal, 2010, 99, 367-376.	0.2	9
150	Molecular Simulation Studies on the Elongation of Gold Nanowires in Benzenedithiol. Journal of Physical Chemistry C, 2010, 114, 10365-10372.	1.5	22
151	Supercritical fluid behavior at nanoscale interfaces: Implications for CO₂sequestration in geologic formations. Philosophical Magazine, 2010, 90, 2339-2363.	0.7	111
152	Direct evidence for fluidâ€“solid transition of nanoconfined fluids. Soft Matter, 2010, 6, 1640.	1.2	32
153	Human Mammary Epithelial Cells Exhibit a Bimodal Correlated Random Walk Pattern. PLoS ONE, 2010, 5, e9636.	1.1	37
154	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
155	Neuroimaging assessment of memoryâ€related brain structures in a rat model of acute spaceâ€like radiation. Journal of Magnetic Resonance Imaging, 2009, 29, 785-792.	1.9	8
156	Bimodal Analysis of Mammary Epithelial Cell Migration in Two Dimensions. Annals of Biomedical Engineering, 2009, 37, 230-245.	1.3	25
157	A molecular dynamics study of the Gibbs free energy of solvation of fullerene particles in octanol and water. Carbon, 2009, 47, 2865-2874.	5.4	30
158	Charging Properties of Cassiterite (Î±-SnO2) Surfaces in NaCl and RbCl Ionic Media. Langmuir, 2009, 25, 10852-10862.	1.6	17
159	Ion Adsorption on Metal Oxide Surfaces to Hydrothermal Conditions.. ECS Transactions, 2008, 11, 167-180.	0.3	7
160	Sintering of titanium dioxide nanoparticles: a comparison between molecular dynamics and phenomenological modeling. Journal of Nanoparticle Research, 2008, 10, 1169-1182.	0.8	49
161	Protrusion of a Virtual Model Lamellipodium by Actin Polymerization: A Coarse-Grained Langevin Dynamics Model. Journal of Statistical Physics, 2008, 133, 79-100.	0.5	8
162	Phase Transformations during Sintering of Titania Nanoparticles. ACS Nano, 2008, 2, 1620-1624.	7.3	96

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163	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
164	Phase coexistence in polydisperse athermal polymer-colloidal mixture. Journal of Chemical Physics, 2008, 128, 154907.	1.2	8
165	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
166	Rate-Dependent Energy Release Mechanism of Gold Nanowires under Elongation. Journal of the American Chemical Society, 2008, 130, 17907-17912.	6.6	19
167	Controlled Translocation of DNA Segments through Nanoelectrode Gaps from Molecular Dynamics. Journal of Physical Chemistry C, 2008, 112, 8-12.	1.5	15
168	Molecular Dynamics Simulation of ss-DNA Translocation between Copper Nanoelectrodes Incorporating Electrode Charge Dynamics. Journal of Physical Chemistry B, 2008, 112, 1712-1717.	1.2	20
169	Electrophoresis of ssDNA through Nanoelectrode Gaps from Molecular Dynamics: Impact of Gap Width and Chain Length. Journal of Physical Chemistry B, 2008, 112, 12851-12858.	1.2	2
170	Adsorption of Water on TiO2 and SnO2 Surfaces: Molecular Dynamics Study. Collection of Czechoslovak Chemical Communications, 2008, 73, 575-589.	1.0	11
171	The importance of polarizability in the modeling of solubility: Quantifying the effect of solute polarizability on the solubility of small nonpolar solutes in popular models of water. Journal of Chemical Physics, 2008, 129, 024508.	1.2	35
172	Effective Interaction Potentials for Coarse-Grained Simulations of Polymer-Tethered Nanoparticle Self-Assembly in Solution. , 2008, , 415-431.		0
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