Jianzhong Wu

List of Publications by Year in descending order

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231 papers	11,677 citations	29994 54 h-index	33814 99 g-index

240 all docs	240 docs citations	240 times ranked	8575 citing authors

#	Article	IF	Citations
1	Anti-Icing Superhydrophobic Coatings. Langmuir, 2009, 25, 12444-12448.	1.6	1,295
2	Structures of hard-sphere fluids from a modified fundamental-measure theory. Journal of Chemical Physics, 2002, 117, 10156-10164.	1.2	601
3	Density functional theory for chemical engineering: From capillarity to soft materials. AICHE Journal, 2006, 52, 1169-1193.	1.8	335
4	Density-Functional Theory for Complex Fluids. Annual Review of Physical Chemistry, 2007, 58, 85-112.	4.8	323
5	Density functional theory for inhomogeneous mixtures of polymeric fluids. Journal of Chemical Physics, 2002, 117, 2368-2376.	1.2	304
6	Oscillation of Capacitance inside Nanopores. Nano Letters, 2011, 11, 5373-5377.	4.5	290
7	Asphaltene precipitation in crude oils: Theory and experiments. AICHE Journal, 2004, 50, 2552-2570.	1.8	245
8	Density-functional theory of spherical electric double layers and Î¶ potentials of colloidal particles in restricted-primitive-model electrolyte solutions. Journal of Chemical Physics, 2004, 120, 7223-7233.	1.2	186
9	Understanding the Electric Double-Layer Structure, Capacitance, and Charging Dynamics. Chemical Reviews, 2022, 122, 10821-10859.	23.0	186
10	Solvent Effect on the Pore-Size Dependence of an Organic Electrolyte Supercapacitor. Journal of Physical Chemistry Letters, 2012, 3, 1727-1731.	2.1	182
11	Computational Insights into Materials and Interfaces for Capacitive Energy Storage. Advanced Science, 2017, 4, 1700059.	5.6	176
12	Molecular-thermodynamic framework for asphaltene-oil equilibria. AICHE Journal, 1998, 44, 1188-1199.	1.8	174
13	A classical density functional theory for interfacial layering of ionic liquids. Soft Matter, 2011, 7, 11222.	1.2	170
14	A fundamental-measure theory for inhomogeneous associating fluids. Journal of Chemical Physics, 2002, 116, 7094-7103.	1.2	169
15	Phase Behavior of Thermally Responsive Microgel Colloids. Physical Review Letters, 2003, 90, 048304.	2.9	162
16	Interaction between like-charged colloidal spheres in electrolyte solutions. Proceedings of the National Academy of Sciences of the United States of America, 1998, 95, 15169-15172.	3.3	154
17	Phase Equilibria for Systems Containing Hydrocarbons, Water, and Salt:Â An Extended Pengâ"Robinson Equation of State. Industrial & Engineering Chemistry Research, 1998, 37, 1634-1643.	1.8	153
18	Enhancing the Capacitive Performance of Electric Double-Layer Capacitors with Ionic Liquid Mixtures. ACS Energy Letters, 2016, 1, 21-26.	8.8	146

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19	Photo-induced ultrafast active ion transport through graphene oxide membranes. Nature Communications, 2019, 10, 1171.	5.8	146
20	Quantum Effects on the Capacitance of Graphene-Based Electrodes. Journal of Physical Chemistry C, 2015, 119, 22297-22303.	1.5	144
21	Density functional theory for differential capacitance of planar electric double layers in ionic liquids. Chemical Physics Letters, 2011, 504, 153-158.	1.2	130
22	Continuous transition from double-layer to Faradaic charge storage in confined electrolytes. Nature Energy, 2022, 7, 222-228.	19.8	130
23	Modeling inhomogeneous van der Waals fluids using an analytical direct correlation function. Physical Review E, 2004, 70, 011201.	0.8	113
24	Microscopic Insights into the Electrochemical Behavior of Nonaqueous Electrolytes in Electric Double-Layer Capacitors. Journal of Physical Chemistry Letters, 2013, 4, 1260-1267.	2.1	113
25	Selective Charging Behavior in an Ionic Mixture Electrolyte-Supercapacitor System for Higher Energy and Power. Journal of the American Chemical Society, 2017, 139, 18681-18687.	6.6	101
26	Assembly of Supertetrahedral T₅ Copperâ"Indium Sulfide Clusters into a Super-Supertetrahedron of Infinite Order. Journal of the American Chemical Society, 2010, 132, 3283-3285.	6.6	99
27	Interparticle Potential and the Phase Behavior of Temperature-Sensitive Microgel Dispersions. Macromolecules, 2003, 36, 440-448.	2.2	94
28	Molecular thermodynamics of asphaltene precipitation in reservoir fluids. AICHE Journal, 2000, 46, 197-209.	1.8	93
29	Membrane-confined liquid-liquid phase separation toward artificial organelles. Science Advances, 2021, 7, .	4.7	89
30	Hunting ionic liquids with large electrochemical potential windows. AICHE Journal, 2019, 65, 804-810.	1.8	83
31	Density Functional Study of the Electric Double Layer Formed by a High Density Electrolyte. Journal of Physical Chemistry B, 2011, 115, 12911-12914.	1.2	81
32	Density functional theory for semiflexible and cyclic polyatomic fluids. Journal of Chemical Physics, 2004, 121, 4210-4220.	1.2	76
33	Insights from machine learning of carbon electrodes for electric double layer capacitors. Carbon, 2020, 157, 147-152.	5.4	74
34	Self-Diffusion of Methane in Single-Walled Carbon Nanotubes at Sub- and Supercritical Conditions. Langmuir, 2004, 20, 3759-3765.	1.6	73
35	A Generic Model for Electric Double Layers in Porous Electrodes. Journal of Physical Chemistry C, 2016, 120, 8704-8710.	1.5	73
36	A Site Density Functional Theory for Water: Application to Solvation of Amino Acid Side Chains. Journal of Chemical Theory and Computation, 2013, 9, 1896-1908.	2.3	72

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37	Density Functional Theory for Polyelectrolytes near Oppositely Charged Surfaces. Physical Review Letters, 2006, 96, 048302.	2.9	71
38	Density Functional Theory for Planar Electric Double Layers:Â Closing the Gap between Simple and Polyelectrolytes. Journal of Physical Chemistry B, 2006, 110, 7473-7484.	1.2	71
39	Polyelectrolyte complex coacervation: Effects of concentration asymmetry. Journal of Chemical Physics, 2018, 149, 163303.	1.2	71
40	Unusual effects of solvent polarity on capacitance for organic electrolytes in a nanoporous electrode. Nanoscale, 2014, 6, 5545-5550.	2.8	70
41	Growth Mechanism of Highly Branched Titanium Dioxide Nanowires via Oriented Attachment. Crystal Growth and Design, 2013, 13, 422-428.	1.4	68
42	Structure and Swelling of Grafted Polyelectrolytes:Â Predictions from a Nonlocal Density Functional Theory. Macromolecules, 2007, 40, 334-343.	2.2	64
43	Extended test-particle method for predicting the inter- and intramolecular correlation functions of polymeric fluids. Journal of Chemical Physics, 2003, 118, 3835-3842.	1.2	63
44	Density-functional theory for the structures and thermodynamic properties of highly asymmetric electrolyte and neutral component mixtures. Physical Review E, 2004, 70, 031109.	0.8	63
45	Salting-Out and Salting-In of Polyelectrolyte Solutions: A Liquid-State Theory Study. Macromolecules, 2016, 49, 9720-9730.	2.2	63
46	Modeling the selectivity of activated carbons for efficient separation of hydrogen and carbon dioxide. Carbon, 2005, 43, 1364-1370.	5.4	62
47	Kinetic Charging Inversion in Ionic Liquid Electric Double Layers. Journal of Physical Chemistry Letters, 2014, 5, 2195-2200.	2.1	62
48	A density-functional theory for bulk and inhomogeneous Lennard-Jones fluids from the energy route. Journal of Chemical Physics, 2003, 119, 7388-7397.	1.2	61
49	Volume transition and internal structures of small poly(N-isopropylacrylamide) microgels. Journal of Polymer Science, Part B: Polymer Physics, 2005, 43, 849-860.	2.4	61
50	Density-functional theory and Monte Carlo simulation for the surface structure and correlation functions of freely jointed Lennard-Jones polymeric fluids. Journal of Chemical Physics, 2005, 122, 174708.	1.2	61
51	Surface Forces between Telechelic Brushes Revisited:Â The Origin of a Weak Attraction. Langmuir, 2006, 22, 2712-2718.	1.6	60
52	New Theoretical Method for Rapid Prediction of Solvation Free Energy in Water. Journal of Physical Chemistry B, 2011, 115, 6971-6975.	1.2	60
53	Microstructure of Block Copolymers near Selective Surfaces:â€‰ Theoretical Predictions and Configurational-Bias Monte Carlo Simulation. Macromolecules, 2005, 38, 971-978.	2.2	58
54	Thermodynamic basis for the genome to capsid charge relationship in viral encapsidation. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 16986-16991.	3.3	56

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55	Protein Refolding Assisted by Periodic Mesoporous Organosilicas. Langmuir, 2007, 23, 5735-5739.	1.6	55
56	Crystallization Kinetics of Thermosensitive Colloids Probed by Transmission Spectroscopy. Langmuir, 2004, 20, 8858-8864.	1.6	54
57	Structures and correlation functions of multicomponent and polydisperse hard-sphere mixtures from a density functional theory. Journal of Chemical Physics, 2004, 121, 1535-1541.	1.2	53
58	Mixed Ionic Liquid Improves Electrolyte Dynamics in Supercapacitors. Journal of Physical Chemistry C, 2018, 122, 10476-10481.	1.5	53
59	Vaporâ"Liquid Equilibria and Interfacial Tensions of Associating Fluids within a Density Functional Theory. Industrial & Engineering Chemistry Research, 2005, 44, 1120-1128.	1.8	51
60	A comprehensive analysis of the BET area for nanoporous materials. AICHE Journal, 2018, 64, 286-293.	1.8	51
61	Forces between aqueous nonuniformly charged colloids from molecular simulation. Journal of Chemical Physics, 2002, 116, 7733-7743.	1.2	50
62	Revisiting density functionals for the primitive model of electric double layers. Journal of Chemical Physics, 2014, 140, 044714.	1.2	50
63	Osmotic pressures of aqueous bovine serum albumin solutions at high ionic strength. Fluid Phase Equilibria, 1999, 155, 139-154.	1.4	48
64	Molecular Simulation of Novel Carbonaceous Materials for Hydrogen Storage. Nano Letters, 2004, 4, 1489-1492.	4.5	47
65	Density Functional Methods for Fast Screening of Metalâ€"Organic Frameworks for Hydrogen Storage. Journal of Physical Chemistry C, 2015, 119, 5374-5385.	1.5	46
66	Orientation-Averaged Pair Potentials between Dipolar Proteins or Colloids. Journal of Physical Chemistry B, 2002, 106, 2714-2720.	1.2	45
67	Time-dependent density functional theory for ion diffusion in electrochemical systems. Journal of Physics Condensed Matter, 2014, 26, 284102.	0.7	45
68	Chemical and Radiation Stability of Ionic Liquids: A Computational Screening Study. Journal of Physical Chemistry C, 2016, 120, 27757-27767.	1.5	45
69	Impurity Effects on Charging Mechanism and Energy Storage of Nanoporous Supercapacitors. Journal of Physical Chemistry C, 2017, 121, 14066-14072.	1.5	45
70	Monte Carlo Simulation for the Double Layer Structure of an Ionic Liquid Using a Dimer Model: A Comparison with the Density Functional Theory. Journal of Physical Chemistry B, 2012, 116, 10364-10370.	1.2	44
71	Electrostatic origins of polyelectrolyte adsorption: Theory and Monte Carlo simulations. Journal of Chemical Physics, 2010, 133, 044906.	1.2	43
72	Effect of the range of attractive interactions on crystallization, metastable phase transition, and percolation in colloidal dispersions. Physical Review E, 2003, 68, 011403.	0.8	42

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73	Pairwise-additive hydrophobic effect for alkanes in water. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 9512-9515.	3.3	42
74	Toward the inverse design of MOF membranes for efficient D2/H2 separation by combination of physics-based and data-driven modeling. Journal of Membrane Science, 2020, 598, 117675.	4.1	42
75	Interaction between oppositely charged micelles or globular proteins. Physical Review E, 2000, 62, 5273-5280.	0.8	41
76	Layering, condensation, and evaporation of short chains in narrow slit pores. Journal of Chemical Physics, 2005, 122, 224701.	1.2	41
77	Application of Density Functional Theory To Study the Double Layer of an Electrolyte with an Explicit Dimer Model for the Solvent. Journal of Physical Chemistry B, 2012, 116, 11356-11361.	1.2	41
78	Time-dependent density functional theory for the charging kinetics of electric double layer containing room-temperature ionic liquids. Journal of Chemical Physics, 2016, 145, 204707.	1.2	41
79	Ionic Effects in Collapse of Polyelectrolyte Brushes. Journal of Physical Chemistry B, 2008, 112, 7713-7720.	1.2	40
80	A hybrid method for predicting the microstructure of polymers with complex architecture: Combination of single-chain simulation with density functional theory. Journal of Chemical Physics, 2006, 124, 164904.	1.2	39
81	Electrochemical Properties of the Double Layer of an Ionic Liquid Using a Dimer Model Electrolyte and Density Functional Theory. Journal of Physical Chemistry B, 2012, 116, 2520-2525.	1.2	38
82	High-Throughput Prediction of the Hydration Free Energies of Small Molecules from a Classical Density Functional Theory. Journal of Physical Chemistry Letters, 2013, 4, 3687-3691.	2.1	37
83	Boosting the Performance of Ionic-Liquid-Based Supercapacitors with Polar Additives. Journal of Physical Chemistry C, 2016, 120, 24041-24047.	1.5	37
84	Structural Transitions of Confined Model Proteins: Molecular Dynamics Simulation and Experimental Validation. Biophysical Journal, 2006, 90, 3224-3238.	0.2	35
85	Excess-Entropy Scaling for Gas Diffusivity in Nanoporous Materials. Langmuir, 2013, 29, 12997-13002.	1.6	35
86	Thermodynamic and Structural Evidence for Reduced Hydrogen Bonding among Water Molecules near Small Hydrophobic Solutes. Journal of Physical Chemistry B, 2015, 119, 12108-12116.	1.2	35
87	A modified fundamental measure theory for spherical particles in microchannels. Journal of Chemical Physics, 2003, 119, 2288-2295.	1.2	34
88	Osmotic Pressure and Packaging Structure of Caged DNA. Biophysical Journal, 2008, 94, 737-746.	0.2	34
89	Classical density functional theory for methane adsorption in metalâ€organic framework materials. AICHE Journal, 2015, 61, 3012-3021.	1.8	34
90	Data-Driven Approach to Understanding the In-Operando Performance of Heteroatom-Doped Carbon Electrodes. ACS Applied Energy Materials, 2020, 3, 5993-6000.	2.5	34

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91	Density functional theory for predicting polymeric forces against surface fouling. Soft Matter, 2010, 6, 4631.	1.2	33
92	Non-Negligible Roles of Pore Size Distribution on Electroosmotic Flow in Nanoporous Materials. ACS Nano, 2019, 13, 8185-8192.	7.3	33
93	Nitrogen-doped porous aromatic frameworks for enhanced CO2 adsorption. Journal of Colloid and Interface Science, 2015, 438, 191-195.	5.0	32
94	A self-consistent approach for modelling the interfacial properties and phase diagrams of Yukawa, Lennard-Jones and square-well fluids. Molecular Physics, 2004, 102, 1479-1488.	0.8	31
95	Surface-induced phase transitions in ultrathin films of block copolymers. Journal of Chemical Physics, 2005, 122, 194703.	1.2	31
96	The tail effect on the shape of an electrical double layer differential capacitance curve. Journal of Chemical Physics, 2013, 138, 144704.	1.2	30
97	Toward a Quantitative Theory of Ultrasmall Liquid Droplets and Vaporî—‚Liquid Nucleation. Industrial & Engineering Chemistry Research, 2008, 47, 4988-4995.	1.8	29
98	Influence of anisotropic ion shape on structure and capacitance of an electric double layer: A Monte Carlo and density functional study. Journal of Chemical Physics, 2013, 139, 054703.	1.2	28
99	Graphene oxide enabled long-term enzymatic transesterification in an anhydrous gas flux. Nature Communications, 2019, 10, 2684.	5.8	28
100	Density functional theory for a primitive model of nanoparticle-block copolymer mixtures. Journal of Chemical Physics, 2007, 126, 144912.	1.2	27
101	Electrostatic Regulation of Genome Packaging in Human Hepatitis B Virus. Biophysical Journal, 2009, 96, 3065-3073.	0.2	27
102	Communication: Long-range angular correlations in liquid water. Journal of Chemical Physics, 2013, 139, 041103.	1.2	27
103	Lectin corona enhances enzymatic catalysis on the surface of magnetic nanoparticles. Biochemical Engineering Journal, 2018, 129, 26-32.	1.8	27
104	Ionic Liquid Mixture Expands the Potential Window and Capacitance of a Supercapacitor in Tandem. Journal of Physical Chemistry C, 2018, 122, 18304-18310.	1.5	27
105	Theoretical Study of Cooperativity in Multivalent Polymers for Colloidal Stabilization. Langmuir, 2005, 21, 9786-9791.	1.6	26
106	A contact-corrected density functional theory for electrolytes at an interface. Physical Chemistry Chemical Physics, 2014, 16, 3934.	1.3	26
107	Molecular Theory for Electrokinetic Transport in pH-Regulated Nanochannels. Journal of Physical Chemistry Letters, 2014, 5, 3015-3020.	2.1	26
108	Melting Kinetics of Thermally Responsive Microgel Crystals. Macromolecules, 2007, 40, 9544-9548.	2.2	25

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109	A theoretical study for nanoparticle partitioning in the lamellae of diblock copolymers. Journal of Chemical Physics, 2008, 128, 074901.	1.2	25
110	Density functional theory study of the capacitance of single file ions in a narrow cylinder. Journal of Colloid and Interface Science, 2015, 449, 130-135.	5.0	25
111	Ion distribution and selectivity of ionic liquids in microporous electrodes. Journal of Chemical Physics, 2017, 146, 174701.	1.2	25
112	Electrolyte cation length influences electrosorption and dynamics in porous carbon supercapacitors. Electrochimica Acta, 2018, 283, 882-893.	2.6	25
113	Overcharging of Nanoparticles in Electrolyte Solutions. Langmuir, 2004, 20, 7333-7338.	1.6	24
114	Potential distribution theorem for the polymer-induced depletion between colloidal particles. Journal of Chemical Physics, 2007, 126, 144904.	1.2	24
115	A perturbative density functional theory for square-well fluids. Journal of Chemical Physics, 2011, 134, 174702.	1.2	24
116	Differential Heat of Adsorption and Isosteres. Langmuir, 2017, 33, 996-1003.	1.6	24
117	Ion association at discretely-charged dielectric interfaces: Giant charge inversion. Journal of Chemical Physics, 2017, 147, 024703.	1.2	24
118	Electric double layer capacitance for ionic liquids in nanoporous electrodes: Effects of pore size and ion composition. Journal of Molecular Liquids, 2018, 270, 145-150.	2.3	24
119	A new perturbation method for electrolyte solutions based on MSA. Fluid Phase Equilibria, 1994, 101, 121-136.	1.4	23
120	A Theoretical Model for the Dynamic Structure of Hepatitis B Nucleocapsid. Biophysical Journal, 2011, 101, 2476-2484.	0.2	23
121	Can ionophobic nanopores enhance the energy storage capacity of electric-double-layer capacitors containing nonaqueous electrolytes?. Journal of Physics Condensed Matter, 2016, 28, 414005.	0.7	23
122	Modeling Surface Charge Regulation of Colloidal Particles in Aqueous Solutions. Langmuir, 2020, 36, 11918-11928.	1.6	23
123	On the hydrophilicity of electrodes for capacitive energy extraction. Journal of Physics Condensed Matter, 2016, 28, 464008.	0.7	22
124	Self-consistent equations governing the dynamics of nonequilibrium colloidal systems. Journal of Chemical Physics, 2011, 134, 054514.	1.2	21
125	Capacitive Energy Extraction by Few-Layer Graphene Electrodes. Journal of Physical Chemistry C, 2017, 121, 14010-14018.	1.5	21
126	Understanding surface charge regulation in silica nanopores. Physical Chemistry Chemical Physics, 2020, 22, 15373-15380.	1.3	21

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127	An efficient method for accurate evaluation of the siteâ€“site direct correlation functions of molecular fluids. Molecular Physics, 2011, 109, 2553-2564.	0.8	20
128	Shape Effect on Nanoparticle Solvation: A Comparison of Morphometric Thermodynamics and Microscopic Theories. Langmuir, 2012, 28, 6997-7006.	1.6	20
129	Seeking metalâ€“organic frameworks for methane storage in natural gas vehicles. Adsorption, 2015, 21, 499-507.	1.4	20
130	Concanavalin A Coated Activated Carbon for High Performance Enzymatic Catalysis. ACS Sustainable Chemistry and Engineering, 2017, 5, 90-96.	3.2	20
131	Cluster formation and bulk phase behavior of colloidal dispersions. Physical Review E, 2009, 80, 021401.	0.8	19
132	Hybrid MCâ^'DFT Method for Studying Multidimensional Entropic Forces. Journal of Physical Chemistry B, 2011, 115, 1450-1460.	1.2	19
133	Molecular density functional theory for multiscale modeling of hydration free energy. Chemical Engineering Science, 2015, 126, 370-382.	1.9	19
134	Molecular thermodynamics for charged biomacromolecules. Fluid Phase Equilibria, 2006, 241, 317-333.	1.4	18
135	Molecular dynamics for the charging behavior of nanostructured electric double layer capacitors containing room temperature ionic liquids. Nano Research, 2015, 8, 931-940.	5.8	18
136	Impurity effects on ionic-liquid-based supercapacitors. Molecular Physics, 2017, 115, 454-464.	0.8	18
137	Structure and capacitance of an electric double layer of an asymmetric valency dimer electrolyte: A comparison of the density functional theory with Monte Carlo simulations. Journal of Molecular Liquids, 2017, 228, 236-242.	2.3	18
138	Separation of long DNA molecules through cleavage of hydrogen bonds under a stretching force. Applied Physics Letters, 2007, 91, .	1.5	17
139	Self-organization of multivalent counterions in polyelectrolyte brushes. Journal of Chemical Physics, 2008, 129, 084903.	1.2	17
140	Equation of State for the Phase Behavior of Carbon Dioxideâ^'Polymer Systems. Industrial & Engineering Chemistry Research, 2010, 49, 7678-7684.	1.8	17
141	Modeling selective ion adsorption into cylindrical nanopores. Chemical Physics Letters, 2018, 709, 116-124.	1.2	17
142	Microscopic insights into the Faradaic reaction effects on the electric double layers. Chemical Engineering Science, 2020, 215, 115452.	1.9	17
143	Modeling Microscopic Morphology and Mechanical Properties of Block Copolymer/Nanoparticle Composites. Macromolecules, 2009, 42, 7537-7544.	2.2	16
144	Solvation of a Spherical Cavity in Simple Liquids: Interpolating between the Limits. Journal of Physical Chemistry B, 2009, 113, 6813-6818.	1.2	16

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145	A molecular theory for optimal blue energy extraction by electrical double layer expansion. Physical Chemistry Chemical Physics, 2015, 17, 23970-23976.	1.3	16
146	Potential of mean force and transient states in polyelectrolyte pair complexation. Journal of Chemical Physics, 2016, 145, 034901.	1.2	16
147	Isotropic-nematic phase transition in athermal solutions of rod-coil diblock copolymers. Journal of Chemical Physics, 2007, 127, 034902.	1.2	15
148	Non-scaling behavior of electroosmotic flow in voltage-gated nanopores. Physical Chemistry Chemical Physics, 2016, 19, 450-457.	1.3	15
149	Demystifying the Stern layer at a metalâ€“electrolyte interface: Local dielectric constant, specific ion adsorption, and partial charge transfer. Journal of Chemical Physics, 2021, 154, 124701.	1.2	15
150	Fast prediction of hydration free energies for SAMPL4 blind test from a classical density functional theory. Journal of Computer-Aided Molecular Design, 2014, 28, 299-304.	1.3	14
151	Partitioning of proteins between an aqueous solution and a weakly-ionizable polyelectrolyte hydrogel. Polymer, 1996, 37, 4803-4808.	1.8	13
152	Self-Amplified Surface Charging and Partitioning of Ionic Liquids in Nanopores. Physical Review Applied, 2017, 8, .	1.5	13
153	Electrochemical Behavior of Nanoporous Supercapacitors with Oligomeric Ionic Liquids. Journal of Physical Chemistry C, 2018, 122, 14402-14407.	1.5	13
154	Entropic forces of single-chain confinement in spherical cavities. Physical Review E, 2010, 82, 041805.	0.8	12
155	A molecular thermodynamic model for the stability of hepatitis B capsids. Journal of Chemical Physics, 2014, 140, 235101.	1.2	12
156	Spreading of a Unilamellar Liposome on Charged Substrates: A Coarse-Grained Molecular Simulation. Langmuir, 2016, 32, 3785-3793.	1.6	12
157	Cation Molecular Structure Affects Mobility and Transport of Electrolytes in Porous Carbons. Journal of the Electrochemical Society, 2019, 166, A507-A514.	1.3	12
158	Generalizations for the Potential of Mean Force between Two Isolated Colloidal Particles from Monte Carlo Simulations. Journal of Colloid and Interface Science, 2002, 252, 326-330.	5.0	11
159	Molecular dynamics for surfactant-assisted protein refolding. Journal of Chemical Physics, 2007, 126, 064906.	1.2	11
160	Dynamic Control of Protein Folding Pathway with a Polymer of Tunable Hydrophobicity. Journal of Physical Chemistry B, 2007, 111, 12303-12309.	1.2	11
161	Structure of an electric double layer containing a 2:2 valency dimer electrolyte. Journal of Colloid and Interface Science, 2015, 449, 175-179.	5.0	11
162	Toward high-throughput predictions of the hydration free energies of small organic molecules from first principles. Fluid Phase Equilibria, 2016, 407, 304-313.	1.4	11

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163	Kinetics of CO₂ diffusion in human carbonic anhydrase: a study using molecular dynamics simulations and the Markov-state model. Physical Chemistry Chemical Physics, 2017, 19, 11690-11697.	1.3	11
164	Thermodynamic Route to Efficient Prediction of Gas Diffusivity in Nanoporous Materials. Langmuir, 2017, 33, 11797-11803.	1.6	11
165	Separation of Carbon Isotopes in Methane with Nanoporous Materials. Industrial & Engineering Chemistry Research, 2018, 57, 5151-5160.	1.8	11
166	Does capillary evaporation limit the accessibility of nonaqueous electrolytes to the ultrasmall pores of carbon electrodes?. Journal of Chemical Physics, 2018, 149, 234708.	1.2	11
167	Side-chain effects on the capacitive behaviour of ionic liquids in microporous electrodes. Molecular Physics, 2019, 117, 3603-3613.	0.8	11
168	Curvature effects on electric-double-layer capacitance. Chinese Journal of Chemical Engineering, 2021, 31, 145-152.	1.7	11
169	Phase equilibria in a system of â€œbreathingâ€•molecules. Fluid Phase Equilibria, 2002, 194-197, 689-700.	1.4	10
170	An improved theoretical procedure for the pore-size analysis of activated carbon by gas adsorption. Chinese Journal of Chemical Engineering, 2018, 26, 551-559.	1.7	10
171	Polyelectrolytes Tailored Enzyme Cascades with Enhanced Stability and Activity for Oneâ€pot Synthesis. ChemCatChem, 2018, 10, 5391-5396.	1.8	10
172	Flow effects on silicate dissolution and ion transport at an aqueous interface. Physical Chemistry Chemical Physics, 2019, 21, 6970-6975.	1.3	10
173	Charge Regulation of Natural Amino Acids in Aqueous Solutions. Journal of Chemical & Engineering Data, 2020, 65, 5630-5642.	1.0	10
174	A GPU implementation of classical density functional theory for rapid prediction of gas adsorption in nanoporous materials. Journal of Chemical Physics, 2020, 153, 074101.	1.2	10
175	Theoretical Insights into MXene Termination and Surface Charge Regulation. Journal of Physical Chemistry C, 2021, 125, 21771-21779.	1.5	10
176	Application of the new perturbation method to predict densities of single electrolyte aqueous solutions. Fluid Phase Equilibria, 1995, 107, 45-59.	1.4	9
177	Structural and dynamic properties of colloids near jamming transition. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2004, 247, 145-151.	2.3	9
178	Gaussian fluctuations in tethered DNA chains. Journal of Chemical Physics, 2011, 134, 065103.	1.2	9
179	Site-site direct correlation functions for three popular molecular models of liquid water. Journal of Chemical Physics, 2013, 139, 064509.	1.2	9
180	An improved classical mapping method for homogeneous electron gases at finite temperature. Journal of Chemical Physics, 2014, 141, 064115.	1.2	9

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181	A Theoretical Study of SRPK Interaction with the Flexible Domains of Hepatitis B Capsids. Biophysical Journal, 2014, 107, 1453-1461.	0.2	9
182	A bridge-functional-based classical mapping method for predicting the correlation functions of uniform electron gases at finite temperature. Journal of Chemical Physics, 2014, 140, 084103.	1.2	9
183	Classical Density Functional Theory for Molecular Systems. Molecular Modeling and Simulation, 2017, , 65-99.	0.2	9
184	Molecular Theory of Hydration at Different Temperatures. Journal of Physical Chemistry B, 2017, 121, 6898-6908.	1.2	9
185	A molecular theory for predicting the thermodynamic efficiency of electrokinetic energy conversion in slit nanochannels. Journal of Chemical Physics, 2018, 148, 084701.	1.2	9
186	Computational screening and design of nanoporous membranes for efficient carbon isotope separation. Green Energy and Environment, 2020, 5, 364-373.	4.7	9
187	Virtual Screening of Nanoporous Materials for Noble Gas Separation. ACS Applied Nano Materials, 2022, 5, 3701-3711.	2.4	9
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