# Jianzhong Wu

## List of Publications by Year in Descending Order



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|---|---|---|---|
| 229 papers | 9,534 citations | 49 h-index | 89 g-index |
| 240 ext. papers | 10,478 ext. citations | 5.1 avg, IF | 6.66 L-index |

| # | Paper | IF | Citations |
|---|---|---|---|
| 229 | Continuous transition from double-layer to Faradaic charge storage in confined electrolytes. *Nature Energy*, **2022**, 7, 222-228 | 62.3 | 15 |
| 228 | Efficient force field and energy emulation through partition of permutationally equivalent atoms.. *Journal of Chemical Physics*, **2022**, 156, 184304 | 3.9 | 1 |
| 227 | Modeling Multicomponent Gas Adsorption in Nanoporous Materials with Two Versions of Nonlocal Classical Density Functional Theory. *Industrial & Engineering Chemistry Research*, **2021**, 60, 17016-17025 | 3.9 | |
| 226 | Ising density functional theory for weak polyelectrolytes with strong coupling of ionization and intrachain correlations.. *Journal of Chemical Physics*, **2021**, 155, 241102 | 3.9 | 0 |
| 225 | Demystifying the Stern layer at a metal-electrolyte interface: Local dielectric constant, specific ion adsorption, and partial charge transfer. *Journal of Chemical Physics*, **2021**, 154, 124701 | 3.9 | 8 |
| 224 | Membrane-confined liquid-liquid phase separation toward artificial organelles. *Science Advances*, **2021**, 7, | 14.3 | 19 |
| 223 | Massively Parallel GPU-Accelerated String Method for Fast and Accurate Prediction of Molecular Diffusivity in Nanoporous Materials. *ACS Applied Nano Materials*, **2021**, 4, 5394-5403 | 5.6 | 1 |
| 222 | Mechanistic Insights of Pore Contributions in Carbon Supercapacitors by Modified Step Potential Electrochemical Spectroscopy. *Journal of the Electrochemical Society*, **2021**, 168, 060530 | 3.9 | 1 |
| 221 | Theoretical insights on the hydration of quinones as catholytes in aqueous redox flow batteries. *Chinese Journal of Chemical Engineering*, **2021**, 37, 72-72 | 3.2 | 0 |
| 220 | Curvature effects on electric-double-layer capacitance. *Chinese Journal of Chemical Engineering*, **2021**, 31, 145-152 | 3.2 | 3 |
| 219 | Thermodynamic non-ideality in charge regulation of weak polyelectrolytes. *Soft Matter*, **2021**, 17, 9221-9234 | 3.4 | 2 |
| 218 | Modeling Nanoporous Materials for the Next Generation of Supercapacitors **2021**, 1-69 | | |
| 217 | Data-Driven Approach to Understanding the In-Operando Performance of Heteroatom-Doped Carbon Electrodes. *ACS Applied Energy Materials*, **2020**, 3, 5993-6000 | 6.1 | 12 |
| 216 | A Multiscale Procedure for Predicting the Hydration Free Energies of Polycyclic Aromatic Hydrocarbons. *Journal of Chemical & Engineering Data*, **2020**, 65, 2206-2211 | 2.8 | 3 |
| 215 | Understanding surface charge regulation in silica nanopores. *Physical Chemistry Chemical Physics*, **2020**, 22, 15373-15380 | 3.6 | 8 |
| 214 | A hybrid theoretical method for predicting electrokinetic energy conversion in nanochannels. *Physical Chemistry Chemical Physics*, **2020**, 22, 9110-9116 | 3.6 | 0 |
| 213 | Wettability of ultra-small pores of carbon electrodes by size-asymmetric ionic fluids. *Journal of Chemical Physics*, **2020**, 152, 054708 | 3.9 | 1 |

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| 212 | Microscopic insights into the Faradaic reaction effects on the electric double layers. *Chemical Engineering Science*, **2020**, 215, 115452 | 4.4 | 7 |
| 211 | 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 | 9.6 | 17 |
| 210 | Computational screening and design of nanoporous membranes for efficient carbon isotope separation. *Green Energy and Environment*, **2020**, 5, 364-373 | 5.7 | 2 |
| 209 | Recent progress in enzymatic functionalization of carbon-hydrogen bonds for the green synthesis of chemicals. *Chinese Journal of Chemical Engineering*, **2020**, 28, 2499-2506 | 3.2 | 0 |
| 208 | Charge Regulation of Natural Amino Acids in Aqueous Solutions. *Journal of Chemical & Engineering Data*, **2020**, 65, 5630-5642 | 2.8 | 3 |
| 207 | Modeling Surface Charge Regulation of Colloidal Particles in Aqueous Solutions. *Langmuir*, **2020**, 36, 11918-11928 | 4 | 9 |
| 206 | A GPU implementation of classical density functional theory for rapid prediction of gas adsorption in nanoporous materials. *Journal of Chemical Physics*, **2020**, 153, 074101 | 3.9 | 4 |
| 205 | Insights from machine learning of carbon electrodes for electric double layer capacitors. *Carbon*, **2020**, 157, 147-152 | 10.4 | 34 |
| 204 | A Diffusion-Reaction Model for One-Pot Synthesis of Chemicals with Enzyme Cascades. *ChemCatChem*, **2020**, 12, 528-535 | 5.2 | 6 |
| 203 | Graphene oxide enabled long-term enzymatic transesterification in an anhydrous gas flux. *Nature Communications*, **2019**, 10, 2684 | 17.4 | 22 |
| 202 | Non-Negligible Roles of Pore Size Distribution on Electroosmotic Flow in Nanoporous Materials. *ACS Nano*, **2019**, 13, 8185-8192 | 16.7 | 24 |
| 201 | 110th Anniversary: Molecular Thermodynamics: An Endless Frontier. *Industrial & Engineering Chemistry Research*, **2019**, 58, 9707-9708 | 3.9 | 1 |
| 200 | Flow effects on silicate dissolution and ion transport at an aqueous interface. *Physical Chemistry Chemical Physics*, **2019**, 21, 6970-6975 | 3.6 | 8 |
| 199 | Photo-induced ultrafast active ion transport through graphene oxide membranes. *Nature Communications*, **2019**, 10, 1171 | 17.4 | 82 |
| 198 | Cation Molecular Structure Affects Mobility and Transport of Electrolytes in Porous Carbons. *Journal of the Electrochemical Society*, **2019**, 166, A507-A514 | 3.9 | 7 |
| 197 | Fractionation of Isotopic Methanes with Metal□Organic Frameworks. *Journal of Physical Chemistry C*, **2019**, 123, 7397-7407 | 3.8 | 4 |
| 196 | Side-chain effects on the capacitive behaviour of ionic liquids in microporous electrodes. *Molecular Physics*, **2019**, 117, 3603-3613 | 1.7 | 5 |
| 195 | Molecular dynamics simulations reveal how graphene oxide stabilizes and activates lipase in an anhydrous gas. *Physical Chemistry Chemical Physics*, **2019**, 21, 25425-25430 | 3.6 | 5 |

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| 194 | Hunting ionic liquids with large electrochemical potential windows. *AICHE Journal*, **2019**, 65, 804-810 | 3.6 | 43 |
| 193 | Mixed Ionic Liquid Improves Electrolyte Dynamics in Supercapacitors. *Journal of Physical Chemistry C*, **2018**, 122, 10476-10481 | 3.8 | 40 |
| 192 | Multimodels computation for adsorption capacity of activated carbon. *Adsorption Science and Technology*, **2018**, 36, 508-520 | 3.6 | 5 |
| 191 | Pluronic-Conjugated Enzyme Cascade for In Situ Oxidation in Biphasic Media. *ChemCatChem*, **2018**, 10, 2003-2008 | 5.2 | 6 |
| 190 | Markov-state model for CO binding with carbonic anhydrase under confinement. *Journal of Chemical Physics*, **2018**, 148, 035101 | 3.9 | 3 |
| 189 | Separation of Carbon Isotopes in Methane with Nanoporous Materials. *Industrial & Engineering Chemistry Research*, **2018**, 57, 5151-5160 | 3.9 | 8 |
| 188 | A molecular theory for predicting the thermodynamic efficiency of electrokinetic energy conversion in slit nanochannels. *Journal of Chemical Physics*, **2018**, 148, 084701 | 3.9 | 7 |
| 187 | A comprehensive analysis of the BET area for nanoporous materials. *AICHE Journal*, **2018**, 64, 286-293 | 3.6 | 32 |
| 186 | An improved theoretical procedure for the pore-size analysis of activated carbon by gas adsorption. *Chinese Journal of Chemical Engineering*, **2018**, 26, 551-559 | 3.2 | 7 |
| 185 | Lectin corona enhances enzymatic catalysis on the surface of magnetic nanoparticles. *Biochemical Engineering Journal*, **2018**, 129, 26-32 | 4.2 | 22 |
| 184 | Polyelectrolyte complex coacervation: Effects of concentration asymmetry. *Journal of Chemical Physics*, **2018**, 149, 163303 | 3.9 | 42 |
| 183 | Electrolyte cation length influences electrosorption and dynamics in porous carbon supercapacitors. *Electrochimica Acta*, **2018**, 283, 882-893 | 6.7 | 15 |
| 182 | Accelerating CO2 Absorption in Aqueous Amine Solutions at High Temperature with Carbonic Anhydrase in Magnetic Nanogels. *Catalysis Letters*, **2018**, 148, 1827-1833 | 2.8 | 3 |
| 181 | Detachment of HCO3− from the Active Site of Carbonic Anhydrase: Molecular Dynamics Simulation and Machine Learning. *Journal of Physical Chemistry C*, **2018**, 122, 20539-20549 | 3.8 | 3 |
| 180 | Modeling selective ion adsorption into cylindrical nanopores. *Chemical Physics Letters*, **2018**, 709, 116-124 | 2.5 | 14 |
| 179 | Ionic Liquid Mixture Expands the Potential Window and Capacitance of a Supercapacitor in Tandem. *Journal of Physical Chemistry C*, **2018**, 122, 18304-18310 | 3.8 | 19 |
| 178 | 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 | 6 | 15 |
| 177 | Does capillary evaporation limit the accessibility of nonaqueous electrolytes to the ultrasmall pores of carbon electrodes?. *Journal of Chemical Physics*, **2018**, 149, 234708 | 3.9 | 9 |

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| 176 | Polyelectrolytes Tailored Enzyme Cascades with Enhanced Stability and Activity for One-pot Synthesis. *ChemCatChem*, **2018**, 10, 5391-5396 | 5.2 | 6 |
| 175 | Electrochemical Behavior of Nanoporous Supercapacitors with Oligomeric Ionic Liquids. *Journal of Physical Chemistry C*, **2018**, 122, 14402-14407 | 3.8 | 7 |
| 174 | Differential Heat of Adsorption and Isosteres. *Langmuir*, **2017**, 33, 996-1003 | 4 | 23 |
| 173 | Computational Insights into Materials and Interfaces for Capacitive Energy Storage. *Advanced Science*, **2017**, 4, 1700059 | 13.6 | 122 |
| 172 | Ion distribution and selectivity of ionic liquids in microporous electrodes. *Journal of Chemical Physics*, **2017**, 146, 174701 | 3.9 | 12 |
| 171 | A theoretical study on the morphological phase diagram of supported lipid bilayers. *Physical Chemistry Chemical Physics*, **2017**, 19, 16897-16903 | 3.6 | 1 |
| 170 | Impurity Effects on Charging Mechanism and Energy Storage of Nanoporous Supercapacitors. *Journal of Physical Chemistry C*, **2017**, 121, 14066-14072 | 3.8 | 27 |
| 169 | Capacitive Energy Extraction by Few-Layer Graphene Electrodes. *Journal of Physical Chemistry C*, **2017**, 121, 14010-14018 | 3.8 | 18 |
| 168 | Kinetics of CO diffusion in human carbonic anhydrase: a study using molecular dynamics simulations and the Markov-state model. *Physical Chemistry Chemical Physics*, **2017**, 19, 11690-11697 | 3.6 | 7 |
| 167 | Classical Density Functional Theory for Molecular Systems. *Molecular Modeling and Simulation*, **2017** , 65-99 | | 5 |
| 166 | Impurity effects on ionic-liquid-based supercapacitors. *Molecular Physics*, **2017**, 115, 454-464 | 1.7 | 13 |
| 165 | Concanavalin A Coated Activated Carbon for High Performance Enzymatic Catalysis. *ACS Sustainable Chemistry and Engineering*, **2017**, 5, 90-96 | 8.3 | 14 |
| 164 | Self-Amplified Surface Charging and Partitioning of Ionic Liquids in Nanopores. *Physical Review Applied*, **2017**, 8, | 4.3 | 9 |
| 163 | Solvation Structure of Surface-Supported Amine Fragments: A Molecular Dynamics Study. *Journal of Physical Chemistry C*, **2017**, 121, 22156-22163 | 3.8 | 3 |
| 162 | Thermodynamic Route to Efficient Prediction of Gas Diffusivity in Nanoporous Materials. *Langmuir*, **2017**, 33, 11797-11803 | 4 | 9 |
| 161 | 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 | 16.4 | 76 |
| 160 | Molecular Theory of Hydration at Different Temperatures. *Journal of Physical Chemistry B*, **2017**, 121, 6898-6908 | 3.4 | 7 |
| 159 | Ion association at discretely-charged dielectric interfaces: Giant charge inversion. *Journal of Chemical Physics*, **2017**, 147, 024703 | 3.9 | 19 |

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| 158 | 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 | 6 | 13 |
| 157 | Square-Gradient Model for Inhomogeneous Systems: From Simple Fluids to Microemulsions, Polymer Blends and Electronic Structure. *Molecular Modeling and Simulation*, **2017**, 31-64 | | 1 |
| 156 | Non-scaling behavior of electroosmotic flow in voltage-gated nanopores. *Physical Chemistry Chemical Physics*, **2016**, 19, 450-457 | 3.6 | 14 |
| 155 | Can ionophobic nanopores enhance the energy storage capacity of electric-double-layer capacitors containing nonaqueous electrolytes?. *Journal of Physics Condensed Matter*, **2016**, 28, 414005 | 1.8 | 20 |
| 154 | Chemical and Radiation Stability of Ionic Liquids: A Computational Screening Study. *Journal of Physical Chemistry C*, **2016**, 120, 27757-27767 | 3.8 | 35 |
| 153 | Molecular Models for Hepatitis B Virus Capsid Formation, Maturation, and Envelopment **2016**, 134-185 | | |
| 152 | Toward high-throughput predictions of the hydration free energies of small organic molecules from first principles. *Fluid Phase Equilibria*, **2016**, 407, 304-313 | 2.5 | 11 |
| 151 | Direct correlation functions for three-site and four-site water models. *Molecular Physics*, **2016**, 114, 2351-2363 | 1.7 | 1 |
| 150 | Predicting hydration free energies of amphetamine-type stimulants with a customized molecular model. *Journal of Physics Condensed Matter*, **2016**, 28, 344001 | 1.8 | 4 |
| 149 | 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 | 3.9 | 33 |
| 148 | Salting-Out and Salting-In of Polyelectrolyte Solutions: A Liquid-State Theory Study. *Macromolecules*, **2016**, 49, 9720-9730 | 5.5 | 42 |
| 147 | Potential of mean force and transient states in polyelectrolyte pair complexation. *Journal of Chemical Physics*, **2016**, 145, 034901 | 3.9 | 10 |
| 146 | Spreading of a Unilamellar Liposome on Charged Substrates: A Coarse-Grained Molecular Simulation. *Langmuir*, **2016**, 32, 3785-93 | 4 | 11 |
| 145 | A Generic Model for Electric Double Layers in Porous Electrodes. *Journal of Physical Chemistry C*, **2016**, 120, 8704-8710 | 3.8 | 57 |
| 144 | Enhancing the Capacitive Performance of Electric Double-Layer Capacitors with Ionic Liquid Mixtures. *ACS Energy Letters*, **2016**, 1, 21-26 | 20.1 | 107 |
| 143 | A life dedicated to the theory of simple fluids In memory of Yiping Tang. *Molecular Physics*, **2016**, 114, 2325-2327 | 1.7 | 1 |
| 142 | On the hydrophilicity of electrodes for capacitive energy extraction. *Journal of Physics Condensed Matter*, **2016**, 28, 464008 | 1.8 | 15 |
| 141 | Boosting the Performance of Ionic-Liquid-Based Supercapacitors with Polar Additives. *Journal of Physical Chemistry C*, **2016**, 120, 24041-24047 | 3.8 | 29 |

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| 140 | Structure of an electric double layer containing a 2:2 valency dimer electrolyte. *Journal of Colloid and Interface Science*, **2015**, 449, 175-9 | 9.3 | 9 |
| 139 | Molecular dynamics for the charging behavior of nanostructured electric double layer capacitors containing room temperature ionic liquids. *Nano Research*, **2015**, 8, 931-940 | 10 | 15 |
| 138 | Theoretic Insights into Porous Carbon-Based Supercapacitors **2015**, 361-378 | | 1 |
| 137 | A Thermodynamic Model for Genome Packaging in Hepatitis B Virus. *Biophysical Journal*, **2015**, 109, 1689-97 | 2.9 | 2 |
| 136 | Seeking metal□organic frameworks for methane storage in natural gas vehicles. *Adsorption*, **2015**, 21, 499-507 | 2.6 | 17 |
| 135 | A molecular theory for optimal blue energy extraction by electrical double layer expansion. *Physical Chemistry Chemical Physics*, **2015**, 17, 23970-6 | 3.6 | 14 |
| 134 | Thermodynamic and Structural Evidence for Reduced Hydrogen Bonding among Water Molecules near Small Hydrophobic Solutes. *Journal of Physical Chemistry B*, **2015**, 119, 12108-16 | 3.4 | 28 |
| 133 | Quantum Effects on the Capacitance of Graphene-Based Electrodes. *Journal of Physical Chemistry C* , **2015**, 119, 22297-22303 | 3.8 | 92 |
| 132 | Molecular density functional theory for multiscale modeling of hydration free energy. *Chemical Engineering Science*, **2015**, 126, 370-382 | 4.4 | 19 |
| 131 | Nitrogen-doped porous aromatic frameworks for enhanced CO2 adsorption. *Journal of Colloid and Interface Science*, **2015**, 438, 191-195 | 9.3 | 30 |
| 130 | Density Functional Methods for Fast Screening of Metal□Organic Frameworks for Hydrogen Storage. *Journal of Physical Chemistry C*, **2015**, 119, 5374-5385 | 3.8 | 38 |
| 129 | Classical density functional theory for methane adsorption in metal-organic framework materials. *AICHE Journal*, **2015**, 61, 3012-3021 | 3.6 | 29 |
| 128 | Density functional theory study of the capacitance of single file ions in a narrow cylinder. *Journal of Colloid and Interface Science*, **2015**, 449, 130-5 | 9.3 | 22 |
| 127 | Revisiting density functionals for the primitive model of electric double layers. *Journal of Chemical Physics*, **2014**, 140, 044714 | 3.9 | 47 |
| 126 | A contact-corrected density functional theory for electrolytes at an interface. *Physical Chemistry Chemical Physics*, **2014**, 16, 3934-8 | 3.6 | 24 |
| 125 | Unusual effects of solvent polarity on capacitance for organic electrolytes in a nanoporous electrode. *Nanoscale*, **2014**, 6, 5545-50 | 7.7 | 58 |
| 124 | Kinetic Charging Inversion in Ionic Liquid Electric Double Layers. *Journal of Physical Chemistry Letters*, **2014**, 5, 2195-200 | 6.4 | 48 |
| 123 | Multiscale simulation of surfactant□aquaporin complex formation and water permeability. *RSC Advances*, **2014**, 4, 37592-37599 | 3.7 | 4 |

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| 122 | A new exchange-correlation functional free of delocalization and static correlation errors. *Physical Chemistry Chemical Physics*, **2014**, 16, 16373-7 | 3.6 | 3 |
| 121 | A molecular thermodynamic model for the stability of hepatitis B capsids. *Journal of Chemical Physics*, **2014**, 140, 235101 | 3.9 | 11 |
| 120 | Molecular Theory for Electrokinetic Transport in pH-Regulated Nanochannels. *Journal of Physical Chemistry Letters*, **2014**, 5, 3015-20 | 6.4 | 23 |
| 119 | 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 | 4.2 | 13 |
| 118 | A theoretical study of SRPK interaction with the flexible domains of hepatitis B capsids. *Biophysical Journal*, **2014**, 107, 1453-61 | 2.9 | 4 |
| 117 | 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 | 3.9 | 8 |
| 116 | Time-dependent density functional theory for ion diffusion in electrochemical systems. *Journal of Physics Condensed Matter*, **2014**, 26, 284102 | 1.8 | 37 |
| 115 | Contact value relations and density functional theory for the electrical double layer. *Molecular Physics*, **2014**, 112, 3144-3151 | 1.7 | 3 |
| 114 | An improved classical mapping method for homogeneous electron gases at finite temperature. *Journal of Chemical Physics*, **2014**, 141, 064115 | 3.9 | 9 |
| 113 | Structure and thermodynamic properties of relativistic electron gases. *Physical Review E*, **2014**, 90, 012141 | 2.4 | 1 |
| 112 | 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 | 3.9 | 27 |
| 111 | Site-site direct correlation functions for three popular molecular models of liquid water. *Journal of Chemical Physics*, **2013**, 139, 064509 | 3.9 | 9 |
| 110 | A liquid-state theory for electron correlation functions and thermodynamics. *Chemical Physics Letters*, **2013**, 556, 336-340 | 2.5 | 5 |
| 109 | Excess-entropy scaling for gas diffusivity in nanoporous materials. *Langmuir*, **2013**, 29, 12997-3002 | 4 | 33 |
| 108 | Communication: Long-range angular correlations in liquid water. *Journal of Chemical Physics*, **2013**, 139, 041103 | 3.9 | 27 |
| 107 | Growth Mechanism of Highly Branched Titanium Dioxide Nanowires via Oriented Attachment. *Crystal Growth and Design*, **2013**, 13, 422-428 | 3.5 | 56 |
| 106 | A Site Density Functional Theory for Water: Application to Solvation of Amino Acid Side Chains. *Journal of Chemical Theory and Computation*, **2013**, 9, 1896-908 | 6.4 | 67 |
| 105 | The tail effect on the shape of an electrical double layer differential capacitance curve. *Journal of Chemical Physics*, **2013**, 138, 144704 | 3.9 | 29 |

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| 104 | Microscopic Insights into the Electrochemical Behavior of Nonaqueous Electrolytes in Electric Double-Layer Capacitors. *Journal of Physical Chemistry Letters*, **2013**, 4, 1260-7 | 6.4 | 95 |
| 103 | Sorting short fragments of single-stranded DNA with an evolving electric double layer. *Journal of Physical Chemistry B*, **2013**, 117, 2267-72 | 3.4 | 6 |
| 102 | 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 | 6.4 | 36 |
| 101 | Solvent Effect on the Pore-Size Dependence of an Organic Electrolyte Supercapacitor. *Journal of Physical Chemistry Letters*, **2012**, 3, 1727-31 | 6.4 | 151 |
| 100 | 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, 2520-5 | 3.4 | 32 |
| 99 | 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, 11356-61 | 3.4 | 30 |
| 98 | Shape effect on nanoparticle solvation: a comparison of morphometric thermodynamics and microscopic theories. *Langmuir*, **2012**, 28, 6997-7006 | 4 | 14 |
| 97 | Density functional theory for encapsidated polyelectrolytes: a comparison with Monte Carlo simulation. *Journal of Chemical Physics*, **2012**, 137, 044905 | 3.9 | 2 |
| 96 | 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, 10364-70 | 3.4 | 38 |
| 95 | A theoretical model for the dynamic structure of hepatitis B nucleocapsid. *Biophysical Journal*, **2011**, 101, 2476-84 | 2.9 | 19 |
| 94 | Oscillation of capacitance inside nanopores. *Nano Letters*, **2011**, 11, 5373-7 | 11.5 | 240 |
| 93 | Separation of single-stranded DNA fragments at a 10-nucleotide resolution by stretching in microfluidic channels. *Lab on A Chip*, **2011**, 11, 4036-40 | 7.2 | 8 |
| 92 | New theoretical method for rapid prediction of solvation free energy in water. *Journal of Physical Chemistry B*, **2011**, 115, 6971-5 | 3.4 | 55 |
| 91 | A classical density functional theory for interfacial layering of ionic liquids. *Soft Matter*, **2011**, 7, 11222 | 3.6 | 143 |
| 90 | Hybrid MC-DFT method for studying multidimensional entropic forces. *Journal of Physical Chemistry B*, **2011**, 115, 1450-60 | 3.4 | 18 |
| 89 | Self-consistent equations governing the dynamics of nonequilibrium colloidal systems. *Journal of Chemical Physics*, **2011**, 134, 054514 | 3.9 | 18 |
| 88 | An efficient method for accurate evaluation of the site-site direct correlation functions of molecular fluids. *Molecular Physics*, **2011**, 109, 2553-2564 | 1.7 | 18 |
| 87 | Density functional study of the electric double layer formed by a high density electrolyte. *Journal of Physical Chemistry B*, **2011**, 115, 12911-4 | 3.4 | 74 |

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| 86 | A theoretical study of colloidal forces near amphiphilic polymer brushes. *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, **2011**, 384, 115-120 | 5.1 | 7 |
| 85 | Density functional theory for differential capacitance of planar electric double layers in ionic liquids. *Chemical Physics Letters*, **2011**, 504, 153-158 | 2.5 | 112 |
| 84 | Gaussian fluctuations in tethered DNA chains. *Journal of Chemical Physics*, **2011**, 134, 065103 | 3.9 | 8 |
| 83 | 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, 16986-91 | 11.5 | 53 |
| 82 | A perturbative density functional theory for square-well fluids. *Journal of Chemical Physics*, **2011**, 134, 174702 | 3.9 | 18 |
| 81 | Electrostatic origins of polyelectrolyte adsorption: Theory and Monte Carlo simulations. *Journal of Chemical Physics*, **2010**, 133, 044906 | 3.9 | 38 |
| 80 | Equation of State for the Phase Behavior of Carbon Dioxide Polymer Systems. *Industrial & Engineering Chemistry Research*, **2010**, 49, 7678-7684 | 3.9 | 17 |
| 79 | Entropic forces of single-chain confinement in spherical cavities. *Physical Review E*, **2010**, 82, 041805 | 2.4 | 10 |
| 78 | Assembly of supertetrahedral T5 copper-indium sulfide clusters into a super-supertetrahedron of infinite order. *Journal of the American Chemical Society*, **2010**, 132, 3283-5 | 16.4 | 93 |
| 77 | Density functional theory for predicting polymeric forces against surface fouling. *Soft Matter*, **2010**, 6, 4631 | 3.6 | 30 |
| 76 | Cluster formation and bulk phase behavior of colloidal dispersions. *Physical Review E*, **2009**, 80, 021401 | 2.4 | 17 |
| 75 | Anti-icing superhydrophobic coatings. *Langmuir*, **2009**, 25, 12444-8 | 4 | 1115 |
| 74 | Modeling Microscopic Morphology and Mechanical Properties of Block Copolymer/Nanoparticle Composites. *Macromolecules*, **2009**, 42, 7537-7544 | 5.5 | 14 |
| 73 | Electrostatic regulation of genome packaging in human hepatitis B virus. *Biophysical Journal*, **2009**, 96, 3065-73 | 2.9 | 23 |
| 72 | Solvation of a spherical cavity in simple liquids: interpolating between the limits. *Journal of Physical Chemistry B*, **2009**, 113, 6813-8 | 3.4 | 15 |
| 71 | Formation of lamellar structures from spherical particles. *Journal of Chemical Physics*, **2009**, 130, 165102 | 3.9 | 6 |
| 70 | Osmotic pressure and packaging structure of caged DNA. *Biophysical Journal*, **2008**, 94, 737-46 | 2.9 | 33 |
| 69 | Ionic effects in collapse of polyelectrolyte brushes. *Journal of Physical Chemistry B*, **2008**, 112, 7713-20 | 3.4 | 35 |

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| 68 | Toward a Quantitative Theory of Ultrasmall Liquid Droplets and Vapor□liquid Nucleation. *Industrial & Engineering Chemistry Research*, **2008**, 47, 4988-4995 | 3.9 | 29 |
| 67 | Pairwise-additive hydrophobic effect for alkanes in water. *Proceedings of the National Academy of Sciences of the United States of America*, **2008**, 105, 9512-5 | 11.5 | 38 |
| 66 | A theoretical study for nanoparticle partitioning in the lamellae of diblock copolymers. *Journal of Chemical Physics*, **2008**, 128, 074901 | 3.9 | 25 |
| 65 | Self-organization of multivalent counterions in polyelectrolyte brushes. *Journal of Chemical Physics*, **2008**, 129, 084903 | 3.9 | 15 |
| 64 | Structure and Swelling of Grafted Polyelectrolytes: Predictions from a Nonlocal Density Functional Theory. *Macromolecules*, **2007**, 40, 334-343 | 5.5 | 56 |
| 63 | Dynamic control of protein folding pathway with a polymer of tunable hydrophobicity. *Journal of Physical Chemistry B*, **2007**, 111, 12303-9 | 3.4 | 11 |
| 62 | Melting Kinetics of Thermally Responsive Microgel Crystals. *Macromolecules*, **2007**, 40, 9544-9548 | 5.5 | 22 |
| 61 | Protein refolding assisted by periodic mesoporous organosilicas. *Langmuir*, **2007**, 23, 5735-9 | 4 | 53 |
| 60 | Molecular dynamics for surfactant-assisted protein refolding. *Journal of Chemical Physics*, **2007**, 126, 064906 | 3.9 | 10 |
| 59 | Density functional theory for a primitive model of nanoparticle-block copolymer mixtures. *Journal of Chemical Physics*, **2007**, 126, 144912 | 3.9 | 27 |
| 58 | Potential distribution theorem for the polymer-induced depletion between colloidal particles. *Journal of Chemical Physics*, **2007**, 126, 144904 | 3.9 | 22 |
| 57 | Separation of long DNA molecules through cleavage of hydrogen bonds under a stretching force. *Applied Physics Letters*, **2007**, 91, 113902 | 3.4 | 14 |
| 56 | Density-functional theory for complex fluids. *Annual Review of Physical Chemistry*, **2007**, 58, 85-112 | 15.7 | 287 |
| 55 | Isotropic-nematic phase transition in athermal solutions of rod-coil diblock copolymers. *Journal of Chemical Physics*, **2007**, 127, 034902 | 3.9 | 15 |
| 54 | Density functional theory for chemical engineering: From capillarity to soft materials. *AICHE Journal*, **2006**, 52, 1169-1193 | 3.6 | 299 |
| 53 | Surface forces between telechelic brushes revisited: the origin of a weak attraction. *Langmuir*, **2006**, 22, 2712-8 | 4 | 59 |
| 52 | 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 | 3.9 | 39 |
| 51 | Structural transitions of confined model proteins: molecular dynamics simulation and experimental validation. *Biophysical Journal*, **2006**, 90, 3224-38 | 2.9 | 35 |

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|---|---|---|---|
| 50 | Density functional theory for polyelectrolytes near oppositely charged surfaces. *Physical Review Letters*, **2006**, 96, 048302 | 7.4 | 67 |
| 49 | Density functional theory for planar electric double layers: closing the gap between simple and polyelectrolytes. *Journal of Physical Chemistry B*, **2006**, 110, 7473-84 | 3.4 | 66 |
| 48 | Molecular thermodynamics for charged biomacromolecules. *Fluid Phase Equilibria*, **2006**, 241, 317-333 | 2.5 | 15 |
| 47 | Layering, condensation, and evaporation of short chains in narrow slit pores. *Journal of Chemical Physics*, **2005**, 122, 224701 | 3.9 | 39 |
| 46 | Vapor□liquid Equilibria and Interfacial Tensions of Associating Fluids within a Density Functional Theory. *Industrial & Engineering Chemistry Research*, **2005**, 44, 1120-1128 | 3.9 | 45 |
| 45 | Theoretical study of cooperativity in multivalent polymers for colloidal stabilization. *Langmuir*, **2005**, 21, 9786-91 | 4 | 26 |
| 44 | Microstructure of Block Copolymers near Selective Surfaces: Theoretical Predictions and Configurational-Bias Monte Carlo Simulation. *Macromolecules*, **2005**, 38, 971-978 | 5.5 | 57 |
| 43 | Modeling the Electrostatics and Size Effect within a Crowded Bioenvironment. *Macromolecular Symposia*, **2005**, 219, 51-58 | 0.8 | 2 |
| 42 | Modeling the selectivity of activated carbons for efficient separation of hydrogen and carbon dioxide. *Carbon*, **2005**, 43, 1364-1370 | 10.4 | 60 |
| 41 | Volume transition and internal structures of small poly(N-isopropylacrylamide) microgels. *Journal of Polymer Science, Part B: Polymer Physics*, **2005**, 43, 849-860 | 2.6 | 57 |
| 40 | 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 | 3.9 | 58 |
| 39 | Surface-induced phase transitions in ultrathin films of block copolymers. *Journal of Chemical Physics* , **2005**, 122, 194703 | 3.9 | 31 |
| 38 | Density functional theory for semiflexible and cyclic polyatomic fluids. *Journal of Chemical Physics*, **2004**, 121, 4210-20 | 3.9 | 75 |
| 37 | Overcharging of nanoparticles in electrolyte solutions. *Langmuir*, **2004**, 20, 7333-8 | 4 | 22 |
| 36 | Crystallization kinetics of thermosensitive colloids probed by transmission spectroscopy. *Langmuir*, **2004**, 20, 8858-64 | 4 | 51 |
| 35 | Asphaltene precipitation in crude oils: Theory and experiments. *AICHE Journal*, **2004**, 50, 2552-2570 | 3.6 | 204 |
| 34 | Structural and dynamic properties of colloids near jamming transition. *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, **2004**, 247, 145-151 | 5.1 | 9 |
| 33 | Jamming phase diagram of colloidal dispersions by molecular dynamics simulations. *Applied Physics Letters*, **2004**, 84, 4565-4567 | 3.4 | 7 |

| | | | |
|---|---|---|---|
| 32 | Self-diffusion of methane in single-walled carbon nanotubes at sub- and supercritical conditions. *Langmuir*, **2004**, 20, 3759-65 | 4 | 67 |
| 31 | Molecular Simulation of Novel Carbonaceous Materials for Hydrogen Storage. *Nano Letters*, **2004**, 4, 1489-1492 | 11.5 | 43 |
| 30 | Modeling inhomogeneous van der Waals fluids using an analytical direct correlation function. *Physical Review E*, **2004**, 70, 011201 | 2.4 | 109 |
| 29 | 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 | 1.7 | 29 |
| 28 | Structures and correlation functions of multicomponent and polydisperse hard-sphere mixtures from a density functional theory. *Journal of Chemical Physics*, **2004**, 121, 1535-41 | 3.9 | 51 |
| 27 | Density-functional theory for the structures and thermodynamic properties of highly asymmetric electrolyte and neutral component mixtures. *Physical Review E*, **2004**, 70, 031109 | 2.4 | 60 |
| 26 | Density-functional theory of spherical electric double layers and zeta potentials of colloidal particles in restricted-primitive-model electrolyte solutions. *Journal of Chemical Physics*, **2004**, 120, 7223-33 | 3.9 | 169 |
| 25 | Interparticle Potential and the Phase Behavior of Temperature-Sensitive Microgel Dispersions. *Macromolecules*, **2003**, 36, 440-448 | 5.5 | 86 |
| 24 | A density-functional theory for bulk and inhomogeneous Lennard-Jones fluids from the energy route. *Journal of Chemical Physics*, **2003**, 119, 7388-7397 | 3.9 | 55 |
| 23 | Extended test-particle method for predicting the inter- and intramolecular correlation functions of polymeric fluids. *Journal of Chemical Physics*, **2003**, 118, 3835-3842 | 3.9 | 63 |
| 22 | A modified fundamental measure theory for spherical particles in microchannels. *Journal of Chemical Physics*, **2003**, 119, 2288-2295 | 3.9 | 32 |
| 21 | Phase behavior of thermally responsive microgel colloids. *Physical Review Letters*, **2003**, 90, 048304 | 7.4 | 148 |
| 20 | Effect of the range of attractive interactions on crystallization, metastable phase transition, and percolation in colloidal dispersions. *Physical Review E*, **2003**, 68, 011403 | 2.4 | 40 |
| 19 | Generalizations for the potential of mean force between two isolated colloidal particles from Monte Carlo simulations. *Journal of Colloid and Interface Science*, **2002**, 252, 326-30 | 9.3 | 9 |
| 18 | Phase equilibria in a system of Breathing molecules. *Fluid Phase Equilibria*, **2002**, 194-197, 689-700 | 2.5 | 8 |
| 17 | Density functional theory for inhomogeneous mixtures of polymeric fluids. *Journal of Chemical Physics*, **2002**, 117, 2368-2376 | 3.9 | 284 |
| 16 | A fundamental-measure theory for inhomogeneous associating fluids. *Journal of Chemical Physics*, **2002**, 116, 7094-7103 | 3.9 | 156 |
| 15 | Orientation-Averaged Pair Potentials between Dipolar Proteins or Colloids. *Journal of Physical Chemistry B*, **2002**, 106, 2714-2720 | 3.4 | 40 |

| | | | |
|---|---|---|---|
| 14 | Forces between aqueous nonuniformly charged colloids from molecular simulation. *Journal of Chemical Physics*, **2002**, 116, 7733-7743 | 3.9 | 48 |
| 13 | Structures of hard-sphere fluids from a modified fundamental-measure theory. *Journal of Chemical Physics*, **2002**, 117, 10156-10164 | 3.9 | 550 |
| 12 | Molecular thermodynamics of asphaltene precipitation in reservoir fluids. *AICHE Journal*, **2000**, 46, 197-209 | 3.6 | 76 |
| 11 | Interaction between oppositely charged micelles or globular proteins. *Physical Review E*, **2000**, 62, 5273-80 | 2.4 | 37 |
| 10 | Osmotic pressures of aqueous bovine serum albumin solutions at high ionic strength. *Fluid Phase Equilibria*, **1999**, 155, 139-154 | 2.5 | 46 |
| 9 | Molecular-thermodynamic framework for asphaltene-oil equilibria. *AICHE Journal*, **1998**, 44, 1188-1199 | 3.6 | 148 |
| 8 | Interaction between like-charged colloidal spheres in electrolyte solutions. *Proceedings of the National Academy of Sciences of the United States of America*, **1998**, 95, 15169-72 | 11.5 | 138 |
| 7 | Phase Equilibria for Systems Containing Hydrocarbons, Water, and Salt: An Extended Peng-Robinson Equation of State. *Industrial & Engineering Chemistry Research*, **1998**, 37, 1634-1643 | 3.9 | 123 |
| 6 | Partitioning of proteins between an aqueous solution and a weakly-ionizable polyelectrolyte hydrogel. *Polymer*, **1996**, 37, 4803-4808 | 3.9 | 10 |
| 5 | Application of the new perturbation method to predict densities of single electrolyte aqueous solutions. *Fluid Phase Equilibria*, **1995**, 107, 45-59 | 2.5 | 9 |
| 4 | A new perturbation method for electrolyte solutions based on MSA. *Fluid Phase Equilibria*, **1994**, 101, 121-136 | 2.5 | 22 |
| 3 | Theoretical Insights into MXene Termination and Surface Charge Regulation. *Journal of Physical Chemistry C*, | 3.8 | 2 |
| 2 | Molecular thermodynamics for amino-acid adsorption at inorganic surfaces. *AICHE Journal*,e17432 | 3.6 | 1 |
| 1 | Understanding the Electric Double-Layer Structure, Capacitance, and Charging Dynamics. *Chemical Reviews*, | 68.1 | 14 |