Edward J Maginn

List of Publications by Year
in descending order

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226 papers	22,274 citations	9234 74 h-index	9073 144 g-index
243 all docs	243 docs citations	243 times ranked	13215 citing authors

#	Article	IF	Citations
1	Why Is CO2So Soluble in Imidazolium-Based Ionic Liquids?. Journal of the American Chemical Society, 2004, 126, 5300-5308.	6.6	1,348
2	Deep Eutectic Solvents: A Review of Fundamentals and Applications. Chemical Reviews, 2021, 121, 1232-1285.	23.0	1,334
3	Ionic liquids: Innovative fluids for chemical processing. AICHE Journal, 2001, 47, 2384-2389.	1.8	1,303
4	Anion Effects on Gas Solubility in Ionic Liquids. Journal of Physical Chemistry B, 2005, 109, 6366-6374.	1.2	920
5	Solubilities and Thermodynamic Properties of Gases in the Ionic Liquid 1-n-Butyl-3-methylimidazolium Hexafluorophosphate. Journal of Physical Chemistry B, 2002, 106, 7315-7320.	1.2	907
6	Molecular Dynamics Study of the Ionic Liquid 1-n-Butyl-3-methylimidazolium Hexafluorophosphate. Journal of Physical Chemistry B, 2002, 106, 12807-12813.	1.2	681
7	Solution Thermodynamics of Imidazolium-Based Ionic Liquids and Water. Journal of Physical Chemistry B, 2001, 105, 10942-10949.	1.2	657
8	Assessing the factors responsible for ionic liquid toxicity to aquatic organisms via quantitative structureâ€“property relationship modeling. Green Chemistry, 2006, 8, 82-90.	4.6	534
9	Amine-Functionalized Task-Specific Ionic Liquids: A Mechanistic Explanation for the Dramatic Increase in Viscosity upon Complexation with CO₂ from Molecular Simulation. Journal of the American Chemical Society, 2008, 130, 14690-14704.	6.6	382
10	Molecular Design of High Capacity, Low Viscosity, Chemically Tunable Ionic Liquids for CO₂ Capture. Journal of Physical Chemistry Letters, 2010, 1, 3494-3499.	2.1	378
11	Liquid Phase Behavior of Imidazolium-Based Ionic Liquids with Alcohols. Journal of Physical Chemistry B, 2004, 108, 5113-5119.	1.2	374
12	Nanoscale design to enable the revolution in renewable energy. Energy and Environmental Science, 2009, 2, 559.	15.6	348
13	Transport diffusivity of methane in silicalite from equilibrium and nonequilibrium simulations. The Journal of Physical Chemistry, 1993, 97, 4173-4181.	2.9	310
14	Measurement of SO2Solubility in Ionic Liquids. Journal of Physical Chemistry B, 2006, 110, 15059-15062.	1.2	310
15	Molecular simulation of ionic liquids: current status and future opportunities. Journal of Physics Condensed Matter, 2009, 21, 373101.	0.7	271
16	Reliable Viscosity Calculation from Equilibrium Molecular Dynamics Simulations: A Time Decomposition Method. Journal of Chemical Theory and Computation, 2015, 11, 3537-3546.	2.3	249
17	Thermodynamic properties of the ionic liquid 1-n-butyl-3-methylimidazolium hexafluorophosphate from Monte Carlo simulations. Green Chemistry, 2002, 4, 112-118.	4.6	239
18	Effect of Temperature and Water Content on the Shear Viscosity of the Ionic Liquid 1-Ethyl-3-methylimidazolium Bis(trifluoromethanesulfonyl)imide As Studied by Atomistic Simulationsâ€. Journal of Physical Chemistry B, 2007, 111, 4867-4876.	1.2	228

#	Article	IF	Citations
19	Molecular Modeling and Experimental Studies of the Thermodynamic and Transport Properties of Pyridinium-Based Ionic Liquids. Journal of Physical Chemistry B, 2006, 110, 2821-2832.	1.2	226
20	Atomistic Simulation of the Thermodynamic and Transport Properties of Ionic Liquids. Accounts of Chemical Research, 2007, 40, 1200-1207.	7.6	225
21	High temperature separation of carbon dioxide/hydrogen mixtures using facilitated supported ionic liquid membranes. Journal of Membrane Science, 2008, 322, 28-31.	4.1	212
22	Direct Correlation between Ionic Liquid Transport Properties and Ion Pair Lifetimes: A Molecular Dynamics Study. Journal of Physical Chemistry Letters, 2015, 6, 700-705.	2.1	211
23	Continuous Fractional Component Monte Carlo:â€‰ An Adaptive Biasing Method for Open System Atomistic Simulations. Journal of Chemical Theory and Computation, 2007, 3, 1451-1463.	2.3	188
24	Thermal and Transport Properties of Six Ionic Liquids: An Experimental and Molecular Dynamics Study. Industrial & Engineering Chemistry Research, 2012, 51, 7242-7254.	1.8	188
25	Atomistic Simulation of the Absorption of Carbon Dioxide and Water in the Ionic Liquid		

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37	Liquid Phase Behavior of Ionic Liquids with Alcohols:Â Experimental Studies and Modeling. Journal of Physical Chemistry B, 2006, 110, 9354-9361.	1.2	133
38	Dynamics of Longn-Alkanes in Silicalite:Â A Hierarchical Simulation Approach. The Journal of Physical Chemistry, 1996, 100, 7155-7173.	2.9	132
39	Heavy Metal Remediation Using Functionalized Mesoporous Silicas with Controlled Macrostructure. Langmuir, 2001, 17, 528-533.	1.6	125
40	A comparison of methods for melting point calculation using molecular dynamics simulations. Journal of Chemical Physics, 2012, 136, 144116.	1.2	125
41	Liquid phase behavior of imidazolium-based ionic liquids with alcohols: effect of hydrogen bonding and non-polar interactions. Fluid Phase Equilibria, 2005, 228-229, 303-309.	1.4	123
42	Absorption of CO2 in the Ionic Liquid 1-n-Hexyl-3-methylimidazolium Tris(pentafluoroethyl)trifluorophosphate ([hmim][FEP]): A Molecular View by Computer Simulations. Journal of Physical Chemistry B, 2009, 113, 7591-7598.	1.2	123
43	Adsorption Studies of Methane, Ethane, and Argon in the Zeolite Mordenite:Â Molecular Simulations and Experiments. Langmuir, 2000, 16, 3823-3834.	1.6	122
44	Molecular Dynamics Simulations of Alkanes in the Zeolite Silicalite:Â Evidence for Resonant Diffusion Effects. Journal of Physical Chemistry B, 1997, 101, 6394-6408.	1.2	117
45	Calculating the Enthalpy of Vaporization for Ionic Liquid Clusters. Journal of Physical Chemistry B, 2007, 111, 9424-9427.	1.2	116
46	¹H NMR and Molecular Dynamics Evidence for an Unexpected Interaction on the Origin of Salting-In/Salting-Out Phenomena. Journal of Physical Chemistry B, 2010, 114, 2004-2014.	1.2	116
47	Amphiphilic interactions of ionic liquids with lipid biomembranes: a molecular simulation study. Soft Matter, 2014, 10, 8641-8651.	1.2	116
48	Best Practices for Computing Transport Properties 1. Self-Diffusivity and Viscosity from Equilibrium Molecular Dynamics [Article v1.0]. Living Journal of Computational Molecular Science, 2020, 2, .	2.2	114
49	A Computational and Experimental Study of the Heat Transfer Properties of Nine Different Ionic Liquids. Journal of Chemical & Engineering Data, 2014, 59, 391-399.	1.0	110
50	Molecular Dynamics Simulations of CO₂ at an Ionic Liquid Interface: Adsorption, Ordering, and Interfacial Crossing. Journal of Physical Chemistry B, 2010, 114, 11827-11837.	1.2	107
51	Photoelectron Spectrum of Isolated Ion-Pairs in Ionic Liquid Vapor. Journal of Physical Chemistry A, 2007, 111, 3191-3195.	1.1	106
52	Cassandra: An open source Monte Carlo package for molecular simulation. Journal of Computational Chemistry, 2017, 38, 1727-1739.	1.5	106
53	Molecular Simulations of Knudsen Wall-slip: Effect of Wall Morphology. Molecular Simulation, 2003, 29, 697-709.	0.9	105
54	Improvement in molecule exchange efficiency in Gibbs ensemble Monte Carlo: Development and implementation of the continuous fractional component move. Journal of Computational Chemistry, 2008, 29, 2520-2530.	1.5	102

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55	Determining the Accuracy of Classical Force Fields for Ionic Liquids: Atomistic Simulation of the Thermodynamic and Transport Properties of 1-Ethyl-3-methylimidazolium Ethylsulfate ([emim][EtSO₄]) and Its Mixtures with Water. Industrial & Engineering Chemistry Research, 2008, 47, 9115-9126.	1.8	102
56	Feasibility of using ionic liquids for carbon dioxide capture. International Journal of Environmental Technology and Management, 2004, 4, 105.	0.1	101
57	Historical Perspective and Current Outlook for Molecular Dynamics As a Chemical Engineering Tool. Industrial & Engineering Chemistry Research, 2010, 49, 3059-3078.	1.8	101
58	System-size corrections for self-diffusion coefficients calculated from molecular dynamics simulations: The case of CO2, n-alkanes, and poly(ethylene glycol) dimethyl ethers. Journal of Chemical Physics, 2016, 145, 074109.	1.2	101
59	Toward a robust and general molecular simulation method for computing solid-liquid coexistence. Journal of Chemical Physics, 2005, 122, 014115.	1.2	100
60	State of Hydrophobic and Hydrophilic Ionic Liquids in Aqueous Solutions: Are the Ions Fully Dissociated?. Journal of Physical Chemistry B, 2013, 117, 12556-12566.	1.2	100
61	What to Do with CO₂. Journal of Physical Chemistry Letters, 2010, 1, 3478-3479.	2.1	98
62	From discovery to data: What must happen for molecular simulation to become a mainstream chemical engineering tool. AICHE Journal, 2009, 55, 1304-1310.	1.8	97
63	Influence of Water on Diffusion in Imidazolium-Based Ionic Liquids: A Pulsed Field Gradient NMR study. Journal of Physical Chemistry B, 2009, 113, 6353-6359.	1.2	97
64	The effect of C2 substitution on melting point and liquid phase dynamics of imidazolium based-ionic liquids: insights from molecular dynamics simulations. Physical Chemistry Chemical Physics, 2012, 14, 12157.	1.3	97
65	Molecular Simulation and Regular Solution Theory Modeling of Pure and Mixed Gas Absorption in the Ionic Liquid 1-n-Hexyl-3-methylimidazolium Bis(Trifluoromethylsulfonyl)amide ([hmim][Tf₂N]). Journal of Physical Chemistry B, 2008, 112, 16710-16720.	1.2	94
66	Transport properties of carbon dioxide and methane from molecular dynamics simulations. Journal of Chemical Physics, 2014, 141, 134101.	1.2	93
67	Molecular mechanisms of ionic liquid cytotoxicity probed by an integrated experimental and computational approach. Scientific Reports, 2016, 6, 19889.	1.6	93
68	Force field comparison and thermodynamic property calculation of supercritical CO2 and CH4 using molecular dynamics simulations. Fluid Phase Equilibria, 2014, 368, 80-90.	1.4	89
69	A Monte Carlo simulation study of the ionic liquid 1-n-butyl-3-methylimidazolium hexafluorophosphate: liquid structure, volumetric properties and infinite dilution solution thermodynamics of CO2. Fluid Phase Equilibria, 2004, 222-223, 195-203.	1.4	85
70	Predicting Infinite-Dilution Activity Coefficients of Organic Solutes in Ionic Liquids. Industrial & Engineering Chemistry Research, 2004, 43, 1039-1048.	1.8	85
71	Molecular simulation of ammonia absorption in the ionic liquid 1â€ethylâ€3â€methylimidazolium bis(trifluoromethylsulfonyl)imide ([emim][Tf₂N]). AICHE Journal, 2009, 55, 2414-2421.	1.8	84
72	Liquid Structure and Transport Properties of the Deep Eutectic Solvent Ethaline. Journal of Physical Chemistry B, 2020, 124, 5251-5264.	1.2	84

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73	Molecular Simulation of Poly-Î±-olefin Synthetic Lubricants:Â Impact of Molecular Architecture on Performance Properties. Journal of Physical Chemistry B, 1999, 103, 10781-10790.	1.2	82
74	Knudsen Diffusivity of a Hard Sphere in a Rough Slit Pore. Physical Review Letters, 2003, 91, 026102.	2.9	79
75	A Force Field for 3,3,3-Fluoro-1-propenes, Including HFO-1234yf. Journal of Physical Chemistry B, 2010, 114, 10133-10142.	1.2	78
76	Impact of Molecular Architecture on the High-Pressure Rheology of Hydrocarbon Fluids. Journal of Physical Chemistry B, 2000, 104, 7774-7783.	1.2	75
77	Beyond Local Solvation Structure: Nanometric Aggregates in Battery Electrolytes and Their Effect on Electrolyte Properties. ACS Energy Letters, 2022, 7, 461-470.	8.8	75
78	Effect of ion structure on conductivity in lithium-doped ionic liquid electrolytes: A molecular dynamics study. Journal of Chemical Physics, 2013, 139, 114508.	1.2	73
79	Computing the melting point and thermodynamic stability of the orthorhombic and monoclinic crystalline polymorphs of the ionic liquid 1-n-butyl-3-methylimidazolium chloride. Journal of Chemical Physics, 2007, 127, 214504.	1.2	72
80	Molecular Dynamics Simulations of Carbon Dioxide and Water at an Ionic Liquid Interface. Journal of Physical Chemistry B, 2011, 115, 10488-10499.	1.2	71
81	Vaporâ€“Liquid Coexistence and Critical Behavior of Ionic Liquids via Molecular Simulations. Journal of Physical Chemistry Letters, 2011, 2, 1439-1443.	2.1	71
82	A general and efficient Monte Carlo method for sampling intramolecular degrees of freedom of branched and cyclic molecules. Journal of Chemical Physics, 2011, 135, 134121.	1.2	70
83	Atomistic simulation of solid-liquid coexistence for molecular systems: Application to triazole and benzene. Journal of Chemical Physics, 2006, 124, 164503.	1.2	69
84	Functionalized Phosphonium Cations Enable Zinc Metal Reversibility in Aqueous Electrolytes. Angewandte Chemie - International Edition, 2021, 60, 12438-12445.	7.2	69
85	Molecular Simulation of the Thermal and Transport Properties of Three Alkali Nitrate Salts. Industrial & Engineering Chemistry Research, 2010, 49, 559-571.	1.8	68
86	Molecular dynamics study of the effect of alkyl chain length on melting points of [C_nMIM][PF₆] ionic liquids. Physical Chemistry Chemical Physics, 2014, 16, 13489-13499.	1.3	68
87	Role of Molecular Modeling in the Development of CO₂â€“Reactive Ionic Liquids. Chemical Reviews, 2018, 118, 5242-5260.	23.0	68
88	Prediction of viscosities and vaporâ€“liquid equilibria for five polyhydric alcohols by molecular simulation. Fluid Phase Equilibria, 2007, 260, 218-231.	1.4	67
89	A method for computing the solubility limit of solids: Application to sodium chloride in water and alcohols. Journal of Chemical Physics, 2010, 133, 124504.	1.2	67
90	Effect of the Surface Energy Barrier on Sorbate Diffusion in AlPO4-5. Journal of Physical Chemistry B, 2001, 105, 2725-2735.	1.2	66

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91	Molecular Mechanism of Ionic-Liquid-Induced Membrane Disruption: Morphological Changes to Bilayers, Multilayers, and Vesicles. Langmuir, 2016, 32, 5403-5411.	1.6	65
92	Limitations and recommendations for the calculation of shear viscosity using reverse nonequilibrium molecular dynamics. Journal of Chemical Physics, 2010, 132, 014103.	1.2	64
93	The solubility of gases in ionic liquids. AICHE Journal, 2017, 63, 4722-4737.	1.8	64
94	Solvation Structure and Dynamics of Li⁺ in Ternary Ionic Liquidâ€“Lithium Salt Electrolytes. Journal of Physical Chemistry B, 2019, 123, 516-527.	1.2	62
95	Ion-Exchange Behavior of One-Dimensional Linked Dodecaniobate Keggin Ion Materials. Chemistry of Materials, 2008, 20, 2513-2521.	3.2	59
96	Critical behaviour and vapour-liquid coexistence of 1-alkyl-3-methylimidazolium bis(trifluoromethylsulfonyl)amide ionic liquidsvia Monte Carlo simulations. Faraday Discussions, 2012, 154, 53-69.	1.6	59
97	Comparison of heterogeneous and homogeneous bubble nucleation using molecular simulations. Physical Review B, 2007, 75, .	1.1	58
98	Structure and Dynamics of Neat and CO₂-Reacted Ionic Liquid Tetrabutylphosphonium 2-Cyanopyrrolide. Industrial & Engineering Chemistry Research, 2011, 50, 8983-8993.	1.8	58
99	Molecular Topology and Local Dynamics Govern the Viscosity of Imidazolium-Based Ionic Liquids. Journal of Physical Chemistry B, 2015, 119, 14934-14944.	1.2	54
100	COSMOâ€RS Calculations of Partition Coefficients: Different Tools for Conformation Search. Chemical Engineering and Technology, 2009, 32, 977-986.	0.9	52
101	Water-in-Salt LiTFSI Aqueous Electrolytes. 1. Liquid Structure from Combined Molecular Dynamics Simulation and Experimental Studies. Journal of Physical Chemistry B, 2021, 125, 4501-4513.	1.2	52
102	Refined Method for Predicting Electrochemical Windows of Ionic Liquids and Experimental Validation Studies. Journal of Physical Chemistry B, 2014, 118, 6250-6255.	1.2	51
103	Pure and binary component sorption equilibria of light hydrocarbons in the zeolite silicalite from grand canonical Monte Carlo simulations. Fluid Phase Equilibria, 1999, 158-160, 19-27.	1.4	50
104	Molecular Modeling of the Vaporâ^'Liquid Equilibrium Properties of the Alternative Refrigerant 2,3,3,3-Tetrafluoro-1-propene (HFO-1234yf). Journal of Physical Chemistry Letters, 2010, 1, 93-96.	2.1	50
105	Efficient viscosity estimation from molecular dynamics simulation via momentum impulse relaxation. Journal of Chemical Physics, 2000, 113, 2079-2087.	1.2	49
106	PyLAT: Python LAMMPS Analysis Tools. Journal of Chemical Information and Modeling, 2019, 59, 1301-1305.	2.5	49
107	Rheology, dynamics, and structure of hydrocarbon blends: a molecular dynamics study of n-hexane/n-hexadecane mixtures. Chemical Engineering Journal, 1999, 74, 129-146.	6.6	48
108	Experimental and Theoretical Methods to Investigate Extraframework Species in a Layered Material of Dodecaniobate Anions. Inorganic Chemistry, 2007, 46, 2067-2079.	1.9	48

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109	Combined Application of High-Field Diffusion NMR and Molecular Dynamics Simulations To Study Dynamics in a Mixture of Carbon Dioxide and an Imidazolium-Based Ionic Liquid. Journal of Physical Chemistry B, 2012, 116, 9141-9151.	1.2	45
110	Water or Anion? Uncovering the Zn²⁺ Solvation Environment in Mixed Zn(TFSI)₂ and LiTFSI Water-in-Salt Electrolytes. ACS Energy Letters, 2021, 6, 3458-3463.	8.8	45
111	Signatures of Ion Pairing and Aggregation in the Vibrational Spectroscopy of Super-Concentrated Aqueous Lithium Bistriflimide Solutions. Journal of Physical Chemistry C, 2020, 124, 3470-3481.	1.5	44
112	Phase Equilibria, Diffusivities, and Equation of State Modeling of HFC-32 and HFC-125 in Imidazolium-Based Ionic Liquids for the Separation of R-410A. Industrial & Engineering Chemistry Research, 2020, 59, 18222-18235.	1.8	43
113	Development and application of effective pairwise potentials for UO2n+, NpO2n+, PuO2n+, and AmO2n+ (n = 1, 2) ions with water. Physical Chemistry Chemical Physics, 2013, 15, 15954.	1.3	42
114	Evolution of microscopic heterogeneity and dynamics in choline chloride-based deep eutectic solvents. Nature Communications, 2022, 13, 219.	5.8	42
115	Small Molecule Solvation Free Energy: Enhanced Conformational Sampling Using Expanded Ensemble Molecular Dynamics Simulation. Journal of Chemical Theory and Computation, 2011, 7, 2910-2918.	2.3	41
116	Thermodynamic Properties of Supercritical Mixtures of Carbon Dioxide and Methane: A Molecular Simulation Study. Journal of Chemical & Engineering Data, 2014, 59, 3041-3054.	1.0	41
117	Reaction Ensemble Monte Carlo Simulation of Complex Molecular Systems. Journal of Chemical Theory and Computation, 2011, 7, 269-279.	2.3	38
118	Force Field Development for Actinyl Ions via Quantum Mechanical Calculations: An Approach to Account for Many Body Solvation Effects. Journal of Physical Chemistry B, 2012, 116, 10885-10897.	1.2	38
119	Materials and Processes for Carbon Capture and Sequestration. ChemSusChem, 2010, 3, 863-864.	3.6	37
120	Molecular Simulation Study of the Solubility, Diffusivity and Permselectivity of Pure and Binary Mixtures of CO₂ and CH₄ in the Ionic Liquid 1-n-Butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide. Industrial & Engineering Chemistry Research, 2015, 54, 8821-8828.	1.8	37
121	Molecular Simulation Study of the Performance of Supported Ionic Liquid Phase Materials for the Separation of Carbon Dioxide from Methane and Hydrogen. Industrial & Engineering Chemistry Research, 2017, 56, 6775-6784.	1.8	37
122	A molecular dynamics study of lithium-containing aprotic heterocyclic ionic liquid electrolytes. Journal of Chemical Physics, 2018, 148, 193834.	1.2	37
123	Structure and Dynamics of Uranyl(VI) and Plutonyl(VI) Cations in Ionic Liquid/Water Mixtures via Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2013, 117, 10852-10868.	1.2	35
124	Water solubility and dynamics of CO2 capture ionic liquids having aprotic heterocyclic anions. Fluid Phase Equilibria, 2014, 368, 72-79.	1.4	33
125	Dynamics of actinyl ions in water: a molecular dynamics simulation study. Physical Chemistry Chemical Physics, 2014, 16, 8060-8069.	1.3	33
126	Predicting the Solubility of Solid Phenanthrene: A Combined Molecular Simulation and Group Contribution Approach. AICHE Journal, 2013, 59, 2647-2661.	1.8	32

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127	Speciation, Conductivities, Diffusivities, and Electrochemical Reduction as a Function of Water Content in Mixtures of Hydrated Chromium Chloride/Choline Chloride. Journal of Physical Chemistry B, 2015, 119, 6018-6023.	1.2	32
128	Molecular Dynamics Simulations of 1-Ethyl-3-methylimidazolium Bis[(trifluoromethyl)sulfonyl]imide Clusters and Nanodrops. Journal of Physical Chemistry A, 2015, 119, 352-368.	1.1	32
129	Solvation Dynamics of Wet Ethaline: Water is the Magic Component. Journal of Physical Chemistry B, 2021, 125, 8888-8901.	1.2	32
130	Monte Carlo simulations of water solubility in ionic liquids: A force field assessment. Fluid Phase Equilibria, 2016, 407, 117-125.	1.4	31
131	Density, local composition and diffusivity of aqueous choline chloride solutions: a molecular dynamics study. Fluid Phase Equilibria, 2004, 217, 97-104.	1.4	30
132	Force field for the atomistic simulation of the properties of hydrazine, organic hydrazine derivatives, and energetic hydrazinium ionic liquids. Pure and Applied Chemistry, 2009, 81, 1799-1828.	0.9	30
133	An MD Study of the Applicability of the Walden Rule and the Nernstâ€“Einstein Model for Ionic Liquids. ChemPhysChem, 2012, 13, 1701-1707.	1.0	30
134	A Nitroxide Containing Organic Molecule in a Deep Eutectic Solvent for Flow Battery Applications. Journal of the Electrochemical Society, 2021, 168, 020527.	1.3	29
135	Machine Learning Directed Optimization of Classical Molecular Modeling Force Fields. Journal of Chemical Information and Modeling, 2021, 61, 4400-4414.	2.5	29
136	Efficient Solvation Free Energy Calculations of Amino Acid Analogs by Expanded Ensemble Molecular Simulation. Journal of Chemical Theory and Computation, 2011, 7, 1394-1403.	2.3	28
137	Computational Design of New Magnesium Electrolytes with Improved Properties. Journal of Physical Chemistry C, 2017, 121, 16126-16136.	1.5	26
138	Water-In-Salt LiTFSI Aqueous Electrolytes (2): Transport Properties and Li⁺ Dynamics Based on Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2021, 125, 13246-13254.	1.2	26
139	An Atomistic Simulation Study of the Role of Asperities and Indentations on Heterogeneous Bubble Nucleation. Journal of Heat Transfer, 2008, 130, .	1.2	25
140	Molecular dynamics investigation of biomimetic ionic liquids. Fluid Phase Equilibria, 2010, 294, 197-205.	1.4	25
141	Molecular Design of High CO₂ Reactivity and Low Viscosity Ionic Liquids for CO₂ Separative Facilitated Transport Membranes. Industrial & Engineering Chemistry Research, 2016, 55, 2821-2830.	1.8	25
142	An elegant access to formation and vaporization enthalpies of ionic liquids by indirect DSC experiment and â€œin silicoâ€•calculations. Chemical Communications, 2012, 48, 6915.	2.2	24
143	Pressure-enthalpy driven molecular dynamics for thermodynamic property calculation II: applications. Fluid Phase Equilibria, 2002, 200, 93-110.	1.4	23
144	Evaluation and Refinement of the General AMBER Force Field for Nineteen Pure Organic Electrolyte Solvents. Journal of Chemical & Engineering Data, 2018, 63, 3488-3502.	1.0	23

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145	Physicochemical Properties of Ionic Liquids. , 0, , 41-126.		22
146	Structure and dynamics of the molten alkali-chloride salts from an X-ray, simulation, and rate theory perspective. Physical Chemistry Chemical Physics, 2020, 22, 22900-22917.	1.3	22
147	Phase Equilibria and Diffusivities of HFC-32 and HFC-125 in Ionic Liquids for the Separation of R-410A. ACS Sustainable Chemistry and Engineering, 2022, 10, 816-830.	3.2	22
148	Molecular Simulation of Polyelectrolye Conformational Dynamics under an AC Electric Field. Macromolecules, 2010, 43, 4805-4813.	2.2	21
149	A comparison of the solvation thermodynamics of amino acid analogues in water, 1-octanol and 1-n-alkyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ionic liquids by molecular simulation. Journal of Chemical Physics, 2012, 137, 184504.	1.2	21
150	A Monte Carlo Simulation Study To Predict the Solubility of Carbon Dioxide, Hydrogen, and Their Mixture in the Ionic Liquids 1-Alkyl-3-methylimidazolium bis(trifluoromethanesulfonyl)amide ([C_nmim⁺][Tf₂N^{â€“}], n = 4, 6). Industrial & Engineering Chemistry Research, 2015, 54, 4385-4395.	1.8	21
151	Impact of confinement on zeolite cracking selectivity via Monte Carlo integration. AICHE Journal, 2000, 46, 2504-2517.	1.8	20
152	How mixing tetraglyme with the ionic liquid 1-n-hexyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide changes volumetric and transport properties: An experimental and computational study. Chemical Engineering Science, 2017, 159, 43-57.	1.9	20
153	Effect of alkyl-group flexibility on the melting point of imidazolium-based ionic liquids. Journal of Chemical Physics, 2020, 153, 044504.	1.2	20
154	Sigma profiles in deep learning: towards a universal molecular descriptor. Chemical Communications, 2022, 58, 5630-5633.	2.2	20
155	A molecular dynamics study of macromolecules in good solvents: Comparison with dielectric spectroscopy experiments. Journal of Chemical Physics, 1998, 109, 5078-5088.	1.2	19
156	Temperature Dependence of Volumetric and Dynamic Properties of Imidazolium-Based Ionic Liquids. Journal of Physical Chemistry B, 2018, 122, 2414-2424.	1.2	19
157	Anion Enhancement at the Liquidâ€“Vacuum Interface of an Ionic Liquid Mixture. Journal of Physical Chemistry C, 2018, 122, 27392-27401.	1.5	19
158	Comparison of fixed charge and polarizable models for predicting the structural, thermodynamic, and transport properties of molten alkali chlorides. Journal of Chemical Physics, 2020, 153, 214502.	1.2	19
159	Deep Eutectic Solvents: A New Class of Versatile Liquids. Journal of Physical Chemistry B, 2020, 124, 11313-11315.	1.2	19
160	Impact of anion shape on Li⁺solvation and on transport properties for lithiumâ€“air batteries: a molecular dynamics study. Physical Chemistry Chemical Physics, 2020, 22, 15842-15852.	1.3	19
161	Refined Classical Force Field for Choline Chloride and Ethylene Glycol Mixtures over Wide Composition Range. Journal of Chemical & Engineering Data, 2022, 67, 1864-1871.	1.0	19
162	Anion Dependent Dynamics and Water Solubility Explained by Hydrogen Bonding Interactions in Mixtures of Water and Aprotic Heterocyclic Anion Ionic Liquids. Journal of Physical Chemistry B, 2016, 120, 12679-12686.	1.2	18

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163	Exchange-Mediated Transport in Battery Electrolytes: Ultrafast or Ultraslow?. Journal of the American Chemical Society, 2022, 144, 8591-8604.	6.6	18
164	Molecular Dynamics Simulations of Polar Polymer Brushes. Macromolecules, 1998, 31, 3116-3129.	2.2	17
165	Pressureâ€“enthalpy driven molecular dynamics for thermodynamic property calculation. Fluid Phase Equilibria, 2002, 200, 75-92.	1.4	17
166	Rapid shear viscosity calculation by momentum impulse relaxation molecular dynamics. Journal of Chemical Physics, 2005, 123, 224904.	1.2	17
167	Predicting the Solubility of the Sparingly Soluble Solids 1,2,4,5-Tetramethylbenzene, Phenanthrene, and Fluorene in Various Organic Solvents by Molecular Simulation. Journal of Chemical & Engineering Data, 2011, 56, 1587-1595.	1.0	17
168	Development of an AMBER-compatible transferable force field for poly(ethylene glycol) ethers (glymes). Journal of Molecular Modeling, 2017, 23, 194.	0.8	17
169	Phase Equilibria of Gases and Liquids with 1-n-butyl-3-Methylimidazolium Tetrafluoroborate. ACS Symposium Series, 2003, , 110-120.	0.5	16
170	Isomolar semigrand ensemble molecular dynamics: Development and application to liquid-liquid equilibria. Journal of Chemical Physics, 2005, 122, 054504.	1.2	16
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