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	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
2	Evolution of microscopic heterogeneity and dynamics in choline chloride-based deep eutectic solvents. Nature Communications, 2022, 13, 219.	5.8	42
3	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
4	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
5	Sigma profiles in deep learning: towards a universal molecular descriptor. Chemical Communications, 2022, 58, 5630-5633.	2.2	20
6	Structure of water-in-salt and water-in-bisalt electrolytes. Physical Chemistry Chemical Physics, 2022, 24, 10727-10736.	1.3	5
7	Ammonium enables reversible aqueous Zn battery chemistries by tailoring the interphase. One Earth, 2022, 5, 413-421.	3.6	10
8	Exchange-Mediated Transport in Battery Electrolytes: Ultrafast or Ultraslow?. Journal of the American Chemical Society, 2022, 144, 8591-8604.	6.6	18
9	Molecular dynamics study of the ionic liquid 1-hexyl-3-methylimidazolium tris(pentafluoroethyl)trifluorophosphate ([<mml:math) Tj ET Q q 1 1 0.784314 rg B1 /Overlock 10 Tf 50 437 Td (xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>f</mml:mi><mml:mi>a</mml:mi><mml:mi>s</mml:mi></mml:math>) From Networked to Isolated: Observing Water Hydrogen Bonds in Concentrated Electrolytes with Two-Dimensional Infrared Spectroscopy. Journal of Physical Chemistry B, 2022, 126, 5305-5319.	1.0	5
10		1.2	9
11	Deep Eutectic Solvents: A Review of Fundamentals and Applications. Chemical Reviews, 2021, 121, 1232-1285.	23.0	1,334
12	Molecular Modeling of the Thermodynamic and Transport Properties of Ionic Liquid-Water Mixtures. , 2021, , 1-5.		0
13	Openâ€source molecular modeling software in chemical engineering focusing on the Molecular Simulation Design Framework. AICHE Journal, 2021, 67, e17206.	1.8	16
14	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
15	Functionalized Phosphonium Cations Enable Zinc Metal Reversibility in Aqueous Electrolytes. Angewandte Chemie - International Edition, 2021, 60, 12438-12445.	7.2	69
16	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
17	Functionalized Phosphonium Cations Enable Zinc Metal Reversibility in Aqueous Electrolytes. Angewandte Chemie, 2021, 133, 12546-12553.	1.6	11
18	MoSDeF Cassandra: A complete Python interface for the Cassandra Monte Carlo software. Journal of Computational Chemistry, 2021, 42, 1321-1331.	1.5	4

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19	Cross-Linking Methodology for Fully Atomistic Models of Hydroxyl-Terminated Polybutadiene and Determination of Mechanical Properties. Macromolecules, 2021, 54, 4488-4496.	2.2	7
20	Solvation Dynamics of Wet Ethaline: Water is the Magic Component. Journal of Physical Chemistry B, 2021, 125, 8888-8901.	1.2	32
21	Machine Learning Directed Optimization of Classical Molecular Modeling Force Fields. Journal of Chemical Information and Modeling, 2021, 61, 4400-4414.	2.5	29
22	Computing the Liquidus of Binary Monatomic Salt Mixtures with Direct Simulation and Alchemical Free Energy Methods. Journal of Physical Chemistry A, 2021, 125, 8498-8513.	1.1	3
23	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
24	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
25	The role of cations in uranyl nanocluster association: a molecular dynamics study. Physical Chemistry Chemical Physics, 2020, 22, 1847-1854.	1.3	0
26	Effect of alkyl-group flexibility on the melting point of imidazolium-based ionic liquids. Journal of Chemical Physics, 2020, 153, 044504.	1.2	20
27	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
28	SEM-Drude Model for the Accurate and Efficient Simulation of MgCl2â€“KCl Mixtures in the Condensed Phase. Journal of Physical Chemistry A, 2020, 124, 7832-7842.	1.1	12
29	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
30	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
31	Deep Eutectic Solvents: A New Class of Versatile Liquids. Journal of Physical Chemistry B, 2020, 124, 11313-11315.	1.2	19
32	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
33	Liquid Structure and Transport Properties of the Deep Eutectic Solvent Ethaline. Journal of Physical Chemistry B, 2020, 124, 5251-5264.	1.2	84
34	Layer-based thermal migration of an ionic liquid nano-droplet on a graphene surface: a molecular dynamics study. Molecular Simulation, 2020, 46, 829-836.	0.9	3
35	Use of a New Size-Weighted Combining Rule to Predict Adsorption in Siliceous Zeolites. Journal of Chemical & Engineering Data, 2020, 65, 1379-1395.	1.0	4
36	Fully Atomistic Molecular Dynamics Simulations of Hydroxyl-Terminated Polybutadiene with Insights into Hydroxyl Aggregation. Macromolecules, 2020, 53, 2594-2605.	2.2	14

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37	Melting points of alkali chlorides evaluated for a polarizable and non-polarizable model. Journal of Chemical Physics, 2020, 153, 011101.	1.2	15
38	Characteristics of Impactful Computational Contributions to The Journal of Physical Chemistry B. Journal of Physical Chemistry B, 2020, 124, 5093-5094.	1.2	3
39	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
40	Thermodynamic properties and fluid phase equilibrium of natural gas containing CO2 and H2O at extreme pressures typically found in pre-salt reservoirs. Journal of Natural Gas Science and Engineering, 2020, 79, 103337.	2.1	8
41	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
42	Prediction of membrane separation efficiency for hydrophobic and hydrophilic proteins. Journal of Molecular Modeling, 2019, 25, 132.	0.8	0
43	PyLAT: Python LAMMPS Analysis Tools. Journal of Chemical Information and Modeling, 2019, 59, 1301-1305.	2.5	49
44	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
45	A molecular dynamics study of lithium-containing aprotic heterocyclic ionic liquid electrolytes. Journal of Chemical Physics, 2018, 148, 193834.	1.2	37
46	Role of Molecular Modeling in the Development of CO₂â€“Reactive Ionic Liquids. Chemical Reviews, 2018, 118, 5242-5260.	23.0	68
47	Temperature Dependence of Volumetric and Dynamic Properties of Imidazolium-Based Ionic Liquids. Journal of Physical Chemistry B, 2018, 122, 2414-2424.	1.2	19
48	Evaluating physical properties of the orthorhombic crystal phase of ammonium perchlorate using a Class II force field. Journal of Chemical Physics, 2018, 149, 244502.	1.2	7
49	Simulation and measurement of water-induced liquid-liquid phase separation of imidazolium ionic liquid mixtures. Journal of Chemical Physics, 2018, 149, 164503.	1.2	5
50	Anion Enhancement at the Liquidâ€“Vacuum Interface of an Ionic Liquid Mixture. Journal of Physical Chemistry C, 2018, 122, 27392-27401.	1.5	19
51	Investigation of the Relationship between Solvation Structure and Battery Performance in Highly Concentrated Aqueous Nitroxy Radical Catholyte. Journal of Physical Chemistry C, 2018, 122, 13815-13826.	1.5	15
52	A molecular dynamics investigation of actinylâ€“ligand speciation in aqueous solution. Physical Chemistry Chemical Physics, 2018, 20, 15753-15763.	1.3	13
53	Hybrid Computational Strategy for Predicting CO₂ Solubilities in Reactive Ionic Liquids. Journal of Physical Chemistry C, 2018, 122, 14213-14221.	1.5	11
54	Reaction Ensemble Monte Carlo Simulations of CO2 Absorption in the Reactive Ionic Liquid Triethyl(octyl)phosphonium 2-Cyanopyrrolide. Journal of Physical Chemistry Letters, 2018, 9, 5213-5218.	2.1	10

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55	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
56	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
57	Influence of Hofmeister Ions on the Structure of Proline-Based Peptide Models: A Combined Experimental and Molecular Modeling Study. Journal of Physical Chemistry B, 2017, 121, 2062-2072.	1.2	7
58	Cassandra: An open source Monte Carlo package for molecular simulation. Journal of Computational Chemistry, 2017, 38, 1727-1739.	1.5	106
59	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
60	Thermodynamic Properties and Fluid Phase Equilibria of Natural Gas Containing CO₂ and H₂O at Extreme Pressures for Injection in the Brazilian Pre-Salt Reservoirs. , 2017, , .		0
61	Discrete Fractional Component Monte Carlo Simulation Study of Dilute Nonionic Surfactants at the Airâ€“Water Interface. Langmuir, 2017, 33, 9793-9802.	1.6	10
62	The solubility of gases in ionic liquids. AICHE Journal, 2017, 63, 4722-4737.	1.8	64
63	Computational Design of New Magnesium Electrolytes with Improved Properties. Journal of Physical Chemistry C, 2017, 121, 16126-16136.	1.5	26
64	Reaction Ensemble Monte Carlo Simulation of Xylene Isomerization in Bulk Phases and under Confinement. Journal of Chemical Theory and Computation, 2017, 13, 4054-4062.	2.3	13
65	Assessing the reliability of computing ion pair lifetimes and self-diffusivity to predict experimental viscosity trends of ionic liquids. Molecular Systems Design and Engineering, 2017, 2, 293-300.	1.7	14
66	Development of an AMBER-compatible transferable force field for poly(ethylene glycol) ethers (glymes). Journal of Molecular Modeling, 2017, 23, 194.	0.8	17
67	Use of molecular dynamics simulations to estimate the solubility of menadione in supercritical CO2 using Chrastil's model. Fluid Phase Equilibria, 2017, 433, 112-118.	1.4	9
68	Molecular mechanisms of ionic liquid cytotoxicity probed by an integrated experimental and computational approach. Scientific Reports, 2016, 6, 19889.	1.6	93
69	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
70	Molecular Mechanism of Ionic-Liquid-Induced Membrane Disruption: Morphological Changes to Bilayers, Multilayers, and Vesicles. Langmuir, 2016, 32, 5403-5411.	1.6	65
71	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
72	Liquid Structure of CO₂â€“Reactive Aprotic Heterocyclic Anion Ionic Liquids from X-ray Scattering and Molecular Dynamics. Journal of Physical Chemistry B, 2016, 120, 11951-11960.	1.2	12

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73	Why are some cyano-based ionic liquids better glucose solvents than water?. Physical Chemistry Chemical Physics, 2016, 18, 18958-18970.	1.3	13
74	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
75	Monte Carlo simulations of water solubility in ionic liquids: A force field assessment. Fluid Phase Equilibria, 2016, 407, 117-125.	1.4	31
76	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
77	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
78	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
79	Molecular Dynamics Simulation Study of the Association of Lidocainium Docusate and Its Derivatives in Aqueous Solution. Molecular Pharmaceutics, 2015, 12, 1893-1901.	2.3	16
80	Monte Carlo simulation and SAFT modeling study of the solvation thermodynamics of dimethylformamide, dimethylsulfoxide, ethanol and 1-propanol in the ionic liquid trimethylbutylammonium bis(trifluoromethylsulfonyl)imide. Physical Chemistry Chemical Physics, 2015, 17, 7449-7462.	1.3	16
81	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
82	The Electrolyte Genome project: A big data approach in battery materials discovery. Computational Materials Science, 2015, 103, 56-67.	1.4	150
83	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
84	Evaluation of the GROMOS 56A_{CARBO} Force Field for the Calculation of Structural, Volumetric, and Dynamic Properties of Aqueous Glucose Systems. Journal of Physical Chemistry B, 2015, 119, 15310-15319.	1.2	14
85	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
86	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
87	Water solubility and dynamics of CO2 capture ionic liquids having aprotic heterocyclic anions. Fluid Phase Equilibria, 2014, 368, 72-79.	1.4	33
88	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
89	Transport properties of carbon dioxide and methane from molecular dynamics simulations. Journal of Chemical Physics, 2014, 141, 134101.	1.2	93
90	Amphiphilic interactions of ionic liquids with lipid biomembranes: a molecular simulation study. Soft Matter, 2014, 10, 8641-8651.	1.2	116

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91	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
92	Dynamics of actinyl ions in water: a molecular dynamics simulation study. Physical Chemistry Chemical Physics, 2014, 16, 8060-8069.	1.3	33
93	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
94	Relationship between Diffusion and Chemical Exchange in Mixtures of Carbon Dioxide and an Amine-Functionalized Ionic Liquid by High Field NMR and Kinetic Monte Carlo Simulations. Journal of Physical Chemistry Letters, 2014, 5, 1766-1770.	2.1	8
95	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
96	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
97	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
98	Predicting the Solubility of Solid Phenanthrene: A Combined Molecular Simulation and Group Contribution Approach. AICHE Journal, 2013, 59, 2647-2661.	1.8	32
99	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
100	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
101	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
102	Toward Fully in Silico Melting Point Prediction Using Molecular Simulations. Journal of Chemical Theory and Computation, 2013, 9, 1592-1599.	2.3	14
103	Making Sense of Enthalpy of Vaporization Trends for Ionic Liquids: New Experimental and Simulation Data Show a Simple Linear Relationship and Help Reconcile Previous Data. Journal of Physical Chemistry B, 2013, 117, 6473-6486.	1.2	158
104	Efficient Estimation of the Equilibrium Solution-Phase Fugacity of Soluble Nonelectrolyte Solids in Binary Solvents by Molecular Simulation. Industrial & Engineering Chemistry Research, 2013, 52, 13743-13760.	1.8	14
105	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
106	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
107	Benchmark Values: Thermochemistry of the Ionic Liquid [C4Py][Cl]. Australian Journal of Chemistry, 2012, 65, 1487.	0.5	16
108	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

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109	A Simple AIMD Approach to Derive Atomic Charges for Condensed Phase Simulation of Ionic Liquids. Journal of Physical Chemistry B, 2012, 116, 10036-10048.	1.2	182
110	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
111	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
112	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
113	A comparison of methods for melting point calculation using molecular dynamics simulations. Journal of Chemical Physics, 2012, 136, 144116.	1.2	125
114	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
115	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
116	Editorial: Ionic Liquids: The Fundamentals and Forces Driving Their Rise. ChemPhysChem, 2012, 13, 1603-1603.	1.0	13
117	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
118	Reaction Ensemble Monte Carlo Simulation of Complex Molecular Systems. Journal of Chemical Theory and Computation, 2011, 7, 269-279.	2.3	38
119	Structure and Dynamics of Neat and CO₂-Reacted Ionic Liquid Tetrabutylphosphonium 2-Cyanopyrrolide. Industrial & Engineering Chemistry Research, 2011, 50, 8983-8993.	1.8	58
120	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
121	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
122	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
123	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
124	A molecular dynamics investigation of the structural and dynamic properties of the ionic liquid 1-n-butyl-3-methylimidazolium bis(trifluoromethanesulfonyl)imide. Journal of Chemical Physics, 2011, 135, 124507.	1.2	172
125	Vaporâ€“Liquid Coexistence and Critical Behavior of Ionic Liquids via Molecular Simulations. Journal of Physical Chemistry Letters, 2011, 2, 1439-1443.	2.1	71
126	Molecular dynamics investigation of biomimetic ionic liquids. Fluid Phase Equilibria, 2010, 294, 197-205.	1.4	25

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127	Materials and Processes for Carbon Capture and Sequestration. ChemSusChem, 2010, 3, 863-864.	3.6	37
128	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
129	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
130	Limitations and recommendations for the calculation of shear viscosity using reverse nonequilibrium molecular dynamics. Journal of Chemical Physics, 2010, 132, 014103.	1.2	64
131	Historical Perspective and Current Outlook for Molecular Dynamics As a Chemical Engineering Tool. Industrial & Engineering Chemistry Research, 2010, 49, 3059-3078.	1.8	101
132	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
133	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
134	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
135	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
136	Molecular Simulation of Polyelectrolye Conformational Dynamics under an AC Electric Field. Macromolecules, 2010, 43, 4805-4813.	2.2	21
137	Molecular Simulation of the Thermal and Transport Properties of Three Alkali Nitrate Salts. Industrial & Engineering Chemistry Research, 2010, 49, 559-571.	1.8	68
138	What to Do with CO₂. Journal of Physical Chemistry Letters, 2010, 1, 3478-3479.	2.1	98
139	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
140	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
141	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
142	COSMOâ€RS Calculations of Partition Coefficients: Different Tools for Conformation Search. Chemical Engineering and Technology, 2009, 32, 977-986.	0.9	52
143	Molecular simulation of ionic liquids: current status and future opportunities. Journal of Physics Condensed Matter, 2009, 21, 373101.	0.7	271
144	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

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145	Nanoscale design to enable the revolution in renewable energy. Energy and Environmental Science, 2009, 2, 559.	15.6	348
146	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
147	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
148	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
149	Atomistic simulation of water adsorption and cation siting in polyoxoniobate materials. Microporous and Mesoporous Materials, 2008, 116, 532-539.	2.2	3
150	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
151	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
152	Atomistic Simulation of the Absorption of Carbon Dioxide and Water in the Ionic Liquid		

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163	Transferable Force Field for Water Adsorption in Cation-Exchanged Titanosilicates. Industrial & Engineering Chemistry Research, 2007, 46, 5754-5765.	1.8	3
164	Atomistic Simulation of the Thermodynamic and Transport Properties of Ionic Liquids. Accounts of Chemical Research, 2007, 40, 1200-1207.	7.6	225
165	Molecular Simulation of Mixtures Containing Imidazolium- and Pyridinium-Based Ionic Liquids and 1-Butanol. ACS Symposium Series, 2007, , 102-125.	0.5	2
166	Prediction of viscosities and vaporâ€“liquid equilibria for five polyhydric alcohols by molecular simulation. Fluid Phase Equilibria, 2007, 260, 218-231.	1.4	67
167	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
168	Monitoring the Synthesis and Composition Analysis of Microsilica Encapsulated Acetylacetonatocarbonyl TriphenylphosphinerhodiumCatalyst by Inductively Coupled Plasma (ICP) Techniques. IEEE Nanotechnology Magazine, 2006, 5, 677-682.	1.1	1
169	Molecular Simulation Study of Some Thermophysical and Transport Properties of Triazolium-Based Ionic Liquids. Journal of Physical Chemistry B, 2006, 110, 18026-18039.	1.2	144
170	Measurement of SO2Solubility in Ionic Liquids. Journal of Physical Chemistry B, 2006, 110, 15059-15062.	1.2	310
171	Atomistic simulation of solid-liquid coexistence for molecular systems: Application to triazole and benzene. Journal of Chemical Physics, 2006, 124, 164503.	1.2	69
172	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
173	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
174	Isomolar-semigrand ensemble molecular dynamics: Application to vapor-liquid equilibrium of the mixture methane/ethane. Journal of Chemical Physics, 2006, 125, 204712.	1.2	7
175	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
176	Phase Equilibria with Gases and Liquids of 1-n-Butyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide. ACS Symposium Series, 2005, , 292-300.	0.5	2
177	Synthesis, Structural Characterization, and Molecular Modeling of Dodecaniobate Keggin Chain Materials.. ChemInform, 2005, 36, no.	0.1	0
178	Isomolar semigrand ensemble molecular dynamics: Development and application to liquid-liquid equilibria. Journal of Chemical Physics, 2005, 122, 054504.	1.2	16
179	Toward a robust and general molecular simulation method for computing solid-liquid coexistence. Journal of Chemical Physics, 2005, 122, 014115.	1.2	100
180	Monte Carlo Simulations of Gas Solubility in the Ionic Liquid 1-n-Butyl-3-methylimidazolium Hexafluorophosphate. Journal of Physical Chemistry B, 2005, 109, 10395-10405.	1.2	166

#	Article	IF	Citations
181	Rapid shear viscosity calculation by momentum impulse relaxation molecular dynamics. Journal of Chemical Physics, 2005, 123, 224904.	1.2	17
182	Synthesis, Structural Characterization, and Molecular Modeling of Dodecaniobate Keggin Chain Materials. Inorganic Chemistry, 2005, 44, 1774-1785.	1.9	136
183	Anion Effects on Gas Solubility in Ionic Liquids. Journal of Physical Chemistry B, 2005, 109, 6366-6374.	1.2	920
184	Feasibility of using ionic liquids for carbon dioxide capture. International Journal of Environmental Technology and Management, 2004, 4, 105.	0.1	101
185	Why Is CO2So Soluble in Imidazolium-Based Ionic Liquids?. Journal of the American Chemical Society, 2004, 126, 5300-5308.	6.6	1,348
186	Density, local composition and diffusivity of aqueous choline chloride solutions: a molecular dynamics study. Fluid Phase Equilibria, 2004, 217, 97-104.	1.4	30
187	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
188	A Molecular Modeling Investigation of Cation and Water Siting in Crystalline Silicotitanates. Journal of Physical Chemistry B, 2004, 108, 17560-17570.	1.2	9
189	Liquid Phase Behavior of Imidazolium-Based Ionic Liquids with Alcohols. Journal of Physical Chemistry B, 2004, 108, 5113-5119.	1.2	374
190	Predicting Infinite-Dilution Activity Coefficients of Organic Solutes in Ionic Liquids. Industrial & Engineering Chemistry Research, 2004, 43, 1039-1048.	1.8	85
191	Phase Equilibria of Gases and Liquids with 1-n-butyl-3-Methylimidazolium Tetrafluoroborate. ACS Symposium Series, 2003, , 110-120.	0.5	16
192	Molecular Structure of Various Ionic Liquids from Gas Phase Ab Initio Calculations. ACS Symposium Series, 2003, , 162-173.	0.5	7
193	Knudsen Diffusivity of a Hard Sphere in a Rough Slit Pore. Physical Review Letters, 2003, 91, 026102.	2.9	79
194	Molecular Simulations of Knudsen Wall-slip: Effect of Wall Morphology. Molecular Simulation, 2003, 29, 697-709.	0.9	105
195	Predicting melting points of quaternary ammonium ionic liquidsElectronic supplementary information (ESI) available: training sets B and C. See http://www.rsc.org/suppdata/gc/b3/b301217d/. Green Chemistry, 2003, 5, 323.	4.6	156
196	Gas Solubilities in 1-n-Butyl-3-methylimidazolium Hexafluorophosphate. ACS Symposium Series, 2002, , 260-269.	0.5	13
197	Pressureâ€“enthalpy driven molecular dynamics for thermodynamic property calculation. Fluid Phase Equilibria, 2002, 200, 75-92.	1.4	17
198	Pressure-enthalpy driven molecular dynamics for thermodynamic property calculation II: applications. Fluid Phase Equilibria, 2002, 200, 93-110.	1.4	23

#	Article	IF	Citations
199	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
200	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
201	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
202	Solution Thermodynamics of Imidazolium-Based Ionic Liquids and Water. Journal of Physical Chemistry B, 2001, 105, 10942-10949.	1.2	657
203	Heavy Metal Remediation Using Functionalized Mesoporous Silicas with Controlled Macrostructure. Langmuir, 2001, 17, 528-533.	1.6	125
204	Effect of the Surface Energy Barrier on Sorbate Diffusion in AlPO4-5. Journal of Physical Chemistry B, 2001, 105, 2725-2735.	1.2	66
205	Ionic liquids: Innovative fluids for chemical processing. AICHE Journal, 2001, 47, 2384-2389.	1.8	1,303
206	A critical comparison of equilibrium, non-equilibrium and boundary-driven molecular dynamics techniques for studying transport in microporous materials. Journal of Chemical Physics, 2001, 115, 8112-8124.	1.2	168
207	Impact of confinement on zeolite cracking selectivity via Monte Carlo integration. AICHE Journal, 2000, 46, 2504-2517.	1.8	20
208	Efficient viscosity estimation from molecular dynamics simulation via momentum impulse relaxation. Journal of Chemical Physics, 2000, 113, 2079-2087.	1.2	49
209	Impact of Molecular Architecture on the High-Pressure Rheology of Hydrocarbon Fluids. Journal of Physical Chemistry B, 2000, 104, 7774-7783.	1.2	75
210	Adsorption Studies of Methane, Ethane, and Argon in the Zeolite Mordenite:Â Molecular Simulations and Experiments. Langmuir, 2000, 16, 3823-3834.	1.6	122
211	A biased grand canonical Monte Carlo method for simulating adsorption using all-atom and branched united atom models. Molecular Physics, 1999, 96, 1375-1390.	0.8	160
212	Molecular dynamics simulations of dielectric relaxation of concentrated polymer solutions. Journal of Chemical Physics, 1999, 111, 1325-1334.	1.2	9
213	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
214	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
215	Dielectric Relaxation of Dipole-Inverted Polar Polymers As Studied by Computer Simulations. Macromolecules, 1999, 32, 6679-6686.	2.2	8
216	Concentration and Size Dependence of Dielectric Strength and Dielectric Relaxation of Polymers in Solutions of a Ï‚ Solvent via Molecular Dynamics Simulations. Macromolecules, 1999, 32, 1284-1292.	2.2	8

#	Article	IF	Citations
217	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
218	Molecular Dynamics Simulations of Polar Polymer Brushes. Macromolecules, 1998, 31, 3116-3129.	2.2	17
219	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
220	Simulation of hydrocarbon diffusion in zeolites. Studies in Surface Science and Catalysis, 1997, 105, 1851-1858.	1.5	5
221	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
222	Dynamics of Longn-Alkanes in Silicalite:Â A Hierarchical Simulation Approach. The Journal of Physical Chemistry, 1996, 100, 7155-7173.	2.9	132
223	Sorption Thermodynamics, Siting, and Conformation of Long n-Alkanes in Silicalite As Predicted by Configurational-Bias Monte Carlo Integration. The Journal of Physical Chemistry, 1995, 99, 2057-2079.	2.9	148
224	Low-Occupancy Sorption Thermodynamics of Long Alkanes in Silicalite Via Molecular Simulation. Studies in Surface Science and Catalysis, 1994, 84, 2099-2105.	1.5	4
225	Transport diffusivity of methane in silicalite from equilibrium and nonequilibrium simulations. The Journal of Physical Chemistry, 1993, 97, 4173-4181.	2.9	310
226	Physicochemical Properties of Ionic Liquids. , 0, , 41-126.		22