Edward J Maginn

List of Publications by Citations

219 papers	18,244 citations	68 h-index	132 g-index
243 ext. papers	20,040 ext. citations	5.1 avg, IF	7.15 L-index

#	Paper	IF	Citations
219	Why Is CO2 so soluble in imidazolium-based ionic liquids?. *Journal of the American Chemical Society*, **2004**, 126, 5300-8	16.4	1213
218	Ionic liquids: Innovative fluids for chemical processing. *AICHE Journal*, **2001**, 47, 2384-2389	3.6	1171
217	Anion effects on gas solubility in ionic liquids. *Journal of Physical Chemistry B*, **2005**, 109, 6366-74	3.4	835
216	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	3.4	829
215	Molecular Dynamics Study of the Ionic Liquid 1-n-Butyl-3-methylimidazolium Hexafluorophosphate. *Journal of Physical Chemistry B*, **2002**, 106, 12807-12813	3.4	638
214	Solution Thermodynamics of Imidazolium-Based Ionic Liquids and Water. *Journal of Physical Chemistry B*, **2001**, 105, 10942-10949	3.4	606
213	Assessing the factors responsible for ionic liquid toxicity to aquatic organisms via quantitative structure-property relationship modeling. *Green Chemistry*, **2006**, 8, 82-90	10	488
212	Deep Eutectic Solvents: A Review of Fundamentals and Applications. *Chemical Reviews*, **2021**, 121, 1232-1285	62.8	358
211	Liquid Phase Behavior of Imidazolium-Based Ionic Liquids with Alcohols. *Journal of Physical Chemistry B*, **2004**, 108, 5113-5119	3.4	355
210	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, 14690-704	16.4	351
209	Molecular Design of High Capacity, Low Viscosity, Chemically Tunable Ionic Liquids for CO2 Capture. *Journal of Physical Chemistry Letters*, **2010**, 1, 3494-3499	6.4	335
208	Nanoscale design to enable the revolution in renewable energy. *Energy and Environmental Science*, **2009**, 2, 559	35.4	311
207	Measurement of SO2 solubility in ionic liquids. *Journal of Physical Chemistry B*, **2006**, 110, 15059-62	3.4	292
206	Transport diffusivity of methane in silicalite from equilibrium and nonequilibrium simulations. *The Journal of Physical Chemistry*, **1993**, 97, 4173-4181		282
205	Molecular simulation of ionic liquids: current status and future opportunities. *Journal of Physics Condensed Matter*, **2009**, 21, 373101	1.8	250
204	Thermodynamic properties of the ionic liquid 1-n-butyl-3-methylimidazolium hexafluorophosphate from Monte Carlo simulations. *Green Chemistry*, **2002**, 4, 112-118	10	226
203	Molecular modeling and experimental studies of the thermodynamic and transport properties of pyridinium-based ionic liquids. *Journal of Physical Chemistry B*, **2006**, 110, 2821-32	3.4	209

202	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 simulations. *Journal of Physical Chemistry B*, **2007**, 111, 4867-76	3.4	207
201	Atomistic simulation of the thermodynamic and transport properties of ionic liquids. *Accounts of Chemical Research*, **2007**, 40, 1200-7	24.3	204
200	High temperature separation of carbon dioxide/hydrogen mixtures using facilitated supported ionic liquid membranes. *Journal of Membrane Science*, **2008**, 322, 28-31	9.6	198
199	Direct Correlation between Ionic Liquid Transport Properties and Ion Pair Lifetimes: A Molecular Dynamics Study. *Journal of Physical Chemistry Letters*, **2015**, 6, 700-5	6.4	171
198	Reliable Viscosity Calculation from Equilibrium Molecular Dynamics Simulations: A Time Decomposition Method. *Journal of Chemical Theory and Computation*, **2015**, 11, 3537-46	6.4	168
197	Atomistic simulation of the absorption of carbon dioxide and water in the ionic liquid 1-n-Hexyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide ([hmim][Tf2N]. *Journal of Physical Chemistry B*, **2008**, 112, 2045-55	3.4	167
196	Continuous Fractional Component Monte Carlo: An Adaptive Biasing Method for Open System Atomistic Simulations. *Journal of Chemical Theory and Computation*, **2007**, 3, 1451-63	6.4	156
195	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	3.9	153
194	Thermal and Transport Properties of Six Ionic Liquids: An Experimental and Molecular Dynamics Study. *Industrial & Engineering Chemistry Research*, **2012**, 51, 7242-7254	3.9	152
193	Monte Carlo simulations of gas solubility in the ionic liquid 1-n-butyl-3-methylimidazolium hexafluorophosphate. *Journal of Physical Chemistry B*, **2005**, 109, 10395-405	3.4	150
192	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	3.9	149
191	A simple AIMD approach to derive atomic charges for condensed phase simulation of ionic liquids. *Journal of Physical Chemistry B*, **2012**, 116, 10036-48	3.4	146
190	Predicting melting points of quaternary ammonium ionic liquids. *Green Chemistry*, **2003**, 5, 323	10	143
189	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, 6473-86	3.4	142
188	A biased grand canonical Monte Carlo method for simulating adsorption using all-atom and branched united atom models. *Molecular Physics*, **1999**, 96, 1375-1390	1.7	141
187	Molecular simulation study of some thermophysical and transport properties of triazolium-based ionic liquids. *Journal of Physical Chemistry B*, **2006**, 110, 18026-39	3.4	135
186	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		134
185	Dynamics of Long n-Alkanes in Silicalite: A Hierarchical Simulation Approach. *The Journal of Physical Chemistry*, **1996**, 100, 7155-7173		129

184	Liquid phase behavior of ionic liquids with alcohols: experimental studies and modeling. *Journal of Physical Chemistry B*, **2006**, 110, 9354-61	3.4	127
183	Synthesis, structural characterization, and molecular modeling of dodecaniobate keggin chain materials. *Inorganic Chemistry*, **2005**, 44, 1774-85	5.1	125
182	The Electrolyte Genome project: A big data approach in battery materials discovery. *Computational Materials Science*, **2015**, 103, 56-67	3.2	123
181	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, 7591-8	3.4	117
180	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	2.5	116
179	Heavy Metal Remediation Using Functionalized Mesoporous Silicas with Controlled Macrostructure. *Langmuir*, **2001**, 17, 528-533	4	115
178	Adsorption Studies of Methane, Ethane, and Argon in the Zeolite Mordenite: Molecular Simulations and Experiments. *Langmuir*, **2000**, 16, 3823-3834	4	114
177	Molecular Dynamics Simulations of Alkanes in the Zeolite Silicalite: Evidence for Resonant Diffusion Effects. *Journal of Physical Chemistry B*, **1997**, 101, 6394-6408	3.4	113
176	Calculating the enthalpy of vaporization for ionic liquid clusters. *Journal of Physical Chemistry B*, **2007**, 111, 9424-7	3.4	110
175	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, 2004-14	3.4	109
174	Photoelectron spectrum of isolated ion-pairs in ionic liquid vapor. *Journal of Physical Chemistry A*, **2007**, 111, 3191-5	2.8	98
173	Molecular Simulations of Knudsen Wall-slip: Effect of Wall Morphology. *Molecular Simulation*, **2003**, 29, 697-709	2	98
172	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	3.9	95
171	A comparison of methods for melting point calculation using molecular dynamics simulations. *Journal of Chemical Physics*, **2012**, 136, 144116	3.9	94
170	Influence of water on diffusion in imidazolium-based ionic liquids: a pulsed field gradient NMR study. *Journal of Physical Chemistry B*, **2009**, 113, 6353-9	3.4	93
169	Amphiphilic interactions of ionic liquids with lipid biomembranes: a molecular simulation study. *Soft Matter*, **2014**, 10, 8641-51	3.6	92
168	A Computational and Experimental Study of the Heat Transfer Properties of Nine Different Ionic Liquids. *Journal of Chemical & Engineering Data*, **2014**, 59, 391-399	2.8	91
167	Molecular dynamics simulations of CO2 at an ionic liquid interface: adsorption, ordering, and interfacial crossing. *Journal of Physical Chemistry B*, **2010**, 114, 11827-37	3.4	90

166	Feasibility of using ionic liquids for carbon dioxide capture. *International Journal of Environmental Technology and Management*, **2004**, 4, 105	0.6	89
165	Historical Perspective and Current Outlook for Molecular Dynamics As a Chemical Engineering Tool. *Industrial & Engineering Chemistry Research*, **2010**, 49, 3059-3078	3.9	86
164	Toward a robust and general molecular simulation method for computing solid-liquid coexistence. *Journal of Chemical Physics*, **2005**, 122, 14115	3.9	85
163	State of hydrophobic and hydrophilic ionic liquids in aqueous solutions: are the ions fully dissociated?. *Journal of Physical Chemistry B*, **2013**, 117, 12556-66	3.4	84
162	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, 16710-20	3.4	84
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160	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, 12157-64	3.6	81
159	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, 2520-30	3.5	81
158	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	2.5	78
157	Predicting Infinite-Dilution Activity Coefficients of Organic Solutes in Ionic Liquids. *Industrial & Engineering Chemistry Research*, **2004**, 43, 1039-1048	3.9	77
156	Knudsen diffusivity of a hard sphere in a rough slit pore. *Physical Review Letters*, **2003**, 91, 026102	7.4	73
155	Molecular mechanisms of ionic liquid cytotoxicity probed by an integrated experimental and computational approach. *Scientific Reports*, **2016**, 6, 19889	4.9	72
154	Molecular simulation of ammonia absorption in the ionic liquid 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ([emim][Tf2N]). *AICHE Journal*, **2009**, 55, 2414-2421	3.6	70
153	Transport properties of carbon dioxide and methane from molecular dynamics simulations. *Journal of Chemical Physics*, **2014**, 141, 134101	3.9	68
152	Molecular Simulation of Poly-□lefin Synthetic Lubricants: Impact of Molecular Architecture on Performance Properties. *Journal of Physical Chemistry B*, **1999**, 103, 10781-10790	3.4	68
151	Force field comparison and thermodynamic property calculation of supercritical CO2 and CH4 using molecular dynamics simulations. *Fluid Phase Equilibria*, **2014**, 368, 80-90	2.5	67
150	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	3.9	66
149	Vapor□liquid Coexistence and Critical Behavior of Ionic Liquids via Molecular Simulations. *Journal of Physical Chemistry Letters*, **2011**, 2, 1439-1443	6.4	65

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145	A force field for 3,3,3-fluoro-1-propenes, including HFO-1234yf. *Journal of Physical Chemistry B*, **2010**, 114, 10133-42	3.4	62
144	Effect of the Surface Energy Barrier on Sorbate Diffusion in AlPO4-5. *Journal of Physical Chemistry B*, **2001**, 105, 2725-2735	3.4	62
143	Molecular dynamics simulations of carbon dioxide and water at an ionic liquid interface. *Journal of Physical Chemistry B*, **2011**, 115, 10488-99	3.4	61
142	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	3.9	60
141	A method for computing the solubility limit of solids: application to sodium chloride in water and alcohols. *Journal of Chemical Physics*, **2010**, 133, 124504	3.9	59
140	From discovery to data: What must happen for molecular simulation to become a mainstream chemical engineering tool. *AICHE Journal*, **2009**, 55, 1304-1310	3.6	59
139	Prediction of viscosities and vapor□quid equilibria for five polyhydric alcohols by molecular simulation. *Fluid Phase Equilibria*, **2007**, 260, 218-231	2.5	58
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136	Best Practices for Computing Transport Properties 1. Self-Diffusivity and Viscosity from Equilibrium Molecular Dynamics [Article v1.0]. *Living Journal of Computational Molecular Science*, **2019**, 1,	10.1	56
135	Molecular Mechanism of Ionic-Liquid-Induced Membrane Disruption: Morphological Changes to Bilayers, Multilayers, and Vesicles. *Langmuir*, **2016**, 32, 5403-11	4	54
134	Limitations and recommendations for the calculation of shear viscosity using reverse nonequilibrium molecular dynamics. *Journal of Chemical Physics*, **2010**, 132, 014103	3.9	53
133	Molecular Simulation of the Thermal and Transport Properties of Three Alkali Nitrate Salts. *Industrial & Engineering Chemistry Research*, **2010**, 49, 559-571	3.9	53
132	Structure and Dynamics of Neat and CO2-Reacted Ionic Liquid Tetrabutylphosphonium 2-Cyanopyrrolide. *Industrial & Engineering Chemistry Research*, **2011**, 50, 8983-8993	3.9	52
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130	Ion-Exchange Behavior of One-Dimensional Linked Dodecaniobate Keggin Ion Materials. *Chemistry of Materials*, **2008**, 20, 2513-2521	9.6	50
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128	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	2.5	49
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124	Liquid Structure and Transport Properties of the Deep Eutectic Solvent Ethaline. *Journal of Physical Chemistry B*, **2020**, 124, 5251-5264	3.4	43
123	COSMO-RS Calculations of Partition Coefficients: Different Tools for Conformation Search. *Chemical Engineering and Technology*, **2009**, 32, 977-986	2	43
122	Experimental and theoretical methods to investigate extraframework species in a layered material of dodecaniobate anions. *Inorganic Chemistry*, **2007**, 46, 2067-79	5.1	43
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119	The solubility of gases in ionic liquids. *AICHE Journal*, **2017**, 63, 4722-4737	3.6	41
118	Molecular Modeling of the Vapor□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	6.4	40
117	Refined method for predicting electrochemical windows of ionic liquids and experimental validation studies. *Journal of Physical Chemistry B*, **2014**, 118, 6250-5	3.4	39
116	Small Molecule Solvation Free Energy: Enhanced Conformational Sampling Using Expanded Ensemble Molecular Dynamics Simulation. *Journal of Chemical Theory and Computation*, **2011**, 7, 2910-8	6.4	37
115	Development and application of effective pairwise potentials for UO2(n+), NpO2(n+), PuO2(n+), and AmO2(n+) (n = 1, 2) ions with water. *Physical Chemistry Chemical Physics*, **2013**, 15, 15954-63	3.6	35
114	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, 10885-97	3.4	35
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112	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	3.9	33
111	Dynamics of actinyl ions in water: a molecular dynamics simulation study. *Physical Chemistry Chemical Physics*, **2014**, 16, 8060-9	3.6	32
110	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, 10852-68	3.4	32
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108	Thermodynamic Properties of Supercritical Mixtures of Carbon Dioxide and Methane: A Molecular Simulation Study. *Journal of Chemical & Engineering Data*, **2014**, 59, 3041-3054	2.8	31
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106	Water solubility and dynamics of CO2 capture ionic liquids having aprotic heterocyclic anions. *Fluid Phase Equilibria*, **2014**, 368, 72-79	2.5	30
105	Predicting the Solubility of Solid Phenanthrene: A Combined Molecular Simulation and Group Contribution Approach. *AICHE Journal*, **2013**, 59, 2647-2661	3.6	29
104	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	2.1	27
103	Density, local composition and diffusivity of aqueous choline chloride solutions: a molecular dynamics study. *Fluid Phase Equilibria*, **2004**, 217, 97-104	2.5	27
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101	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	3.8	26
100	A molecular dynamics study of lithium-containing aprotic heterocyclic ionic liquid electrolytes. *Journal of Chemical Physics*, **2018**, 148, 193834	3.9	26
99	Efficient Solvation Free Energy Calculations of Amino Acid Analogs by Expanded Ensemble Molecular Simulation. *Journal of Chemical Theory and Computation*, **2011**, 7, 1394-403	6.4	26
98	Monte Carlo simulations of water solubility in ionic liquids: A force field assessment. *Fluid Phase Equilibria*, **2016**, 407, 117-125	2.5	25
97	PyLAT: Python LAMMPS Analysis Tools. *Journal of Chemical Information and Modeling*, **2019**, 59, 1301-1305	5.1	25
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95	Molecular dynamics investigation of biomimetic ionic liquids. *Fluid Phase Equilibria*, **2010**, 294, 197-205	2.5	23

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89	An elegant access to formation and vaporization enthalpies of ionic liquids by indirect DSC experiment and "in silico" calculations. *Chemical Communications*, **2012**, 48, 6915-7	5.8	21
88	An Atomistic Simulation Study of the Role of Asperities and Indentations on Heterogeneous Bubble Nucleation. *Journal of Heat Transfer*, **2008**, 130,	1.8	20
87	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	4.4	19
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 ([Cnmim+][Tf2N‖ n = 4, 6). *Industrial & Engineering Chemistry Research*, **2015**, 54, 4385-4395	3.9	18
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80	Isomolar semigrand ensemble molecular dynamics: development and application to liquid-liquid equilibria. *Journal of Chemical Physics*, **2005**, 122, 54504	3.9	16
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75	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	2.8	15
74	Pressure□nthalpy driven molecular dynamics for thermodynamic property calculation. *Fluid Phase Equilibria*, **2002**, 200, 75-92	2.5	15
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69	Development of an AMBER-compatible transferable force field for poly(ethylene glycol) ethers (glymes). *Journal of Molecular Modeling*, **2017**, 23, 194	2	14
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60	Effect of alkyl-group flexibility on the melting point of imidazolium-based ionic liquids. *Journal of Chemical Physics*, **2020**, 153, 044504	3.9	11
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