Edward J Maginn

List of Publications by Year in Descending Order

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	Evolution of microscopic heterogeneity and dynamics in choline chloride-based deep eutectic solvents.. *Nature Communications*, **2022**, 13, 219	17.4	3
218	Beyond Local Solvation Structure: Nanometric Aggregates in Battery Electrolytes and Their Effect on Electrolyte Properties. *ACS Energy Letters*, **2022**, 7, 461-470	20.1	11
217	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	8.3	2
216	Ammonium enables reversible aqueous Zn battery chemistries by tailoring the interphase. *One Earth*, **2022**, 5, 413-421	8.1	2
215	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	3.4	4
214	Functionalized Phosphonium Cations Enable Zinc Metal Reversibility in Aqueous Electrolytes. *Angewandte Chemie - International Edition*, **2021**, 60, 12438-12445	16.4	23
213	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	3.4	16
212	Functionalized Phosphonium Cations Enable Zinc Metal Reversibility in Aqueous Electrolytes. *Angewandte Chemie*, **2021**, 133, 12546-12553	3.6	1
211	MoSDeF Cassandra: A complete Python interface for the Cassandra Monte Carlo software. *Journal of Computational Chemistry*, **2021**, 42, 1321-1331	3.5	2
210	Cross-Linking Methodology for Fully Atomistic Models of Hydroxyl-Terminated Polybutadiene and Determination of Mechanical Properties. *Macromolecules*, **2021**, 54, 4488-4496	5.5	3
209	Deep Eutectic Solvents: A Review of Fundamentals and Applications. *Chemical Reviews*, **2021**, 121, 1232-1285	62.8	358
208	Open-source molecular modeling software in chemical engineering focusing on the Molecular Simulation Design Framework. *AICHE Journal*, **2021**, 67, e17206	3.6	6
207	A Nitroxide Containing Organic Molecule in a Deep Eutectic Solvent for Flow Battery Applications. *Journal of the Electrochemical Society*, **2021**, 168, 020527	3.9	8
206	Solvation Dynamics of Wet Ethaline: Water is the Magic Component. *Journal of Physical Chemistry B* , **2021**, 125, 8888-8901	3.4	7
205	Machine Learning Directed Optimization of Classical Molecular Modeling Force Fields. *Journal of Chemical Information and Modeling*, **2021**, 61, 4400-4414	6.1	5
204	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	2.8	0
203	Deep Eutectic Solvents: A New Class of Versatile Liquids. *Journal of Physical Chemistry B*, **2020**, 124, 11334-11345	3.4	55

202	Impact of anion shape on Li solvation and on transport properties for lithium-air batteries: a molecular dynamics study. *Physical Chemistry Chemical Physics*, **2020**, 22, 15842-15852	3.6	11
201	Liquid Structure and Transport Properties of the Deep Eutectic Solvent Ethaline. *Journal of Physical Chemistry B*, **2020**, 124, 5251-5264	3.4	43
200	Layer-based thermal migration of an ionic liquid nano-droplet on a graphene surface: a molecular dynamics study. *Molecular Simulation*, **2020**, 46, 829-836	2	2
199	Use of a New Size-Weighted Combining Rule to Predict Adsorption in Siliceous Zeolites. *Journal of Chemical & Engineering Data*, **2020**, 65, 1379-1395	2.8	2
198	Fully Atomistic Molecular Dynamics Simulations of Hydroxyl-Terminated Polybutadiene with Insights into Hydroxyl Aggregation. *Macromolecules*, **2020**, 53, 2594-2605	5.5	5
197	Melting points of alkali chlorides evaluated for a polarizable and non-polarizable model. *Journal of Chemical Physics*, **2020**, 153, 011101	3.9	7
196	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
195	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	4.6	1
194	The role of cations in uranyl nanocluster association: a molecular dynamics study. *Physical Chemistry Chemical Physics*, **2020**, 22, 1847-1854	3.6	
193	Effect of alkyl-group flexibility on the melting point of imidazolium-based ionic liquids. *Journal of Chemical Physics*, **2020**, 153, 044504	3.9	11
192	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	3.9	15
191	SEM-Drude Model for the Accurate and Efficient Simulation of MgCl-KCl Mixtures in the Condensed Phase. *Journal of Physical Chemistry A*, **2020**, 124, 7832-7842	2.8	4
190	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	3.6	8
189	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	3.9	7
188	Prediction of membrane separation efficiency for hydrophobic and hydrophilic proteins : A coarse-grained Brownian dynamics simulation study. *Journal of Molecular Modeling*, **2019**, 25, 132	2	
187	PyLAT: Python LAMMPS Analysis Tools. *Journal of Chemical Information and Modeling*, **2019**, 59, 1301-1305	5.1	25
186	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
185	Solvation Structure and Dynamics of Li in Ternary Ionic Liquid-Lithium Salt Electrolytes. *Journal of Physical Chemistry B*, **2019**, 123, 516-527	3.4	35

184	A molecular dynamics study of lithium-containing aprotic heterocyclic ionic liquid electrolytes. *Journal of Chemical Physics*, **2018**, 148, 193834	3.9	26
183	Role of Molecular Modeling in the Development of CO-Reactive Ionic Liquids. *Chemical Reviews*, **2018**, 118, 5242-5260	68.1	47
182	Temperature Dependence of Volumetric and Dynamic Properties of Imidazolium-Based Ionic Liquids. *Journal of Physical Chemistry B*, **2018**, 122, 2414-2424	3.4	14
181	Reaction Ensemble Monte Carlo Simulations of CO Absorption in the Reactive Ionic Liquid Triethyl(octyl)phosphonium 2-Cyanopyrrolide. *Journal of Physical Chemistry Letters*, **2018**, 9, 5213-5218	6.4	9
180	Evaluation and Refinement of the General AMBER Force Field for Nineteen Pure Organic Electrolyte Solvents. *Journal of Chemical & Engineering Data*, **2018**, 63, 3488-3502	2.8	13
179	Evaluating physical properties of the orthorhombic crystal phase of ammonium perchlorate using a Class II force field. *Journal of Chemical Physics*, **2018**, 149, 244502	3.9	3
178	Simulation and measurement of water-induced liquid-liquid phase separation of imidazolium ionic liquid mixtures. *Journal of Chemical Physics*, **2018**, 149, 164503	3.9	3
177	Anion Enhancement at the Liquid□Vacuum Interface of an Ionic Liquid Mixture. *Journal of Physical Chemistry C*, **2018**, 122, 27392-27401	3.8	16
176	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	3.8	9
175	A molecular dynamics investigation of actinyl-ligand speciation in aqueous solution. *Physical Chemistry Chemical Physics*, **2018**, 20, 15753-15763	3.6	8
174	Hybrid Computational Strategy for Predicting CO2 Solubilities in Reactive Ionic Liquids. *Journal of Physical Chemistry C*, **2018**, 122, 14213-14221	3.8	8
173	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
172	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	3.4	6
171	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
170	Discrete Fractional Component Monte Carlo Simulation Study of Dilute Nonionic Surfactants at the Air-Water Interface. *Langmuir*, **2017**, 33, 9793-9802	4	7
169	The solubility of gases in ionic liquids. *AICHE Journal*, **2017**, 63, 4722-4737	3.6	41
168	Computational Design of New Magnesium Electrolytes with Improved Properties. *Journal of Physical Chemistry C*, **2017**, 121, 16126-16136	3.8	21
167	Reaction Ensemble Monte Carlo Simulation of Xylene Isomerization in Bulk Phases and under Confinement. *Journal of Chemical Theory and Computation*, **2017**, 13, 4054-4062	6.4	12

166	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	4.6	10
165	Development of an AMBER-compatible transferable force field for poly(ethylene glycol) ethers (glymes). *Journal of Molecular Modeling*, **2017**, 23, 194	2	14
164	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	2.5	6
163	Monte Carlo simulations of water solubility in ionic liquids: A force field assessment. *Fluid Phase Equilibria*, **2016**, 407, 117-125	2.5	25
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	3.4	15
161	Liquid Structure of CO-Reactive Aprotic Heterocyclic Anion Ionic Liquids from X-ray Scattering and Molecular Dynamics. *Journal of Physical Chemistry B*, **2016**, 120, 11951-11960	3.4	8
160	Why are some cyano-based ionic liquids better glucose solvents than water?. *Physical Chemistry Chemical Physics*, **2016**, 18, 18958-70	3.6	11
159	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	3.9	21
158	Molecular mechanisms of ionic liquid cytotoxicity probed by an integrated experimental and computational approach. *Scientific Reports*, **2016**, 6, 19889	4.9	72
157	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
156	Molecular Mechanism of Ionic-Liquid-Induced Membrane Disruption: Morphological Changes to Bilayers, Multilayers, and Vesicles. *Langmuir*, **2016**, 32, 5403-11	4	54
155	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
154	Molecular dynamics simulation study of the association of lidocainium docusate and its derivatives in aqueous solution. *Molecular Pharmaceutics*, **2015**, 12, 1893-901	5.6	9
153	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*,	3.6	9
152	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, 6018-23	3.4	26
151	The Electrolyte Genome project: A big data approach in battery materials discovery. *Computational Materials Science*, **2015**, 103, 56-67	3.2	123
150	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	3.9	31
149	Evaluation of the GROMOS 56ACARBO Force Field for the Calculation of Structural, Volumetric, and Dynamic Properties of Aqueous Glucose Systems. *Journal of Physical Chemistry B*, **2015**, 119, 15310-9	3.4	10

148	Molecular dynamics simulations of 1-ethyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide clusters and nanodrops. *Journal of Physical Chemistry A*, **2015**, 119, 352-68	2.8	21
147	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
146	Molecular Topology and Local Dynamics Govern the Viscosity of Imidazolium-Based Ionic Liquids. *Journal of Physical Chemistry B*, **2015**, 119, 14934-44	3.4	44
145	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
144	Water solubility and dynamics of CO2 capture ionic liquids having aprotic heterocyclic anions. *Fluid Phase Equilibria*, **2014**, 368, 72-79	2.5	30
143	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
142	Molecular Simulation of Ionic Liquids: Where We Are and the Path Forward **2014**, 149-192		4
141	Transport properties of carbon dioxide and methane from molecular dynamics simulations. *Journal of Chemical Physics*, **2014**, 141, 134101	3.9	68
140	Amphiphilic interactions of ionic liquids with lipid biomembranes: a molecular simulation study. *Soft Matter*, **2014**, 10, 8641-51	3.6	92
139	Molecular dynamics study of the effect of alkyl chain length on melting points of [CnMIM][PF6] ionic liquids. *Physical Chemistry Chemical Physics*, **2014**, 16, 13489-99	3.6	56
138	Dynamics of actinyl ions in water: a molecular dynamics simulation study. *Physical Chemistry Chemical Physics*, **2014**, 16, 8060-9	3.6	32
137	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
136	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, 1766-70	6.4	8
135	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
134	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
133	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
132	Predicting the Solubility of Solid Phenanthrene: A Combined Molecular Simulation and Group Contribution Approach. *AICHE Journal*, **2013**, 59, 2647-2661	3.6	29
131	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

130	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
129	Effect of ion structure on conductivity in lithium-doped ionic liquid electrolytes: a molecular dynamics study. *Journal of Chemical Physics*, **2013**, 139, 114508	3.9	62
128	Toward Fully in Silico Melting Point Prediction Using Molecular Simulations. *Journal of Chemical Theory and Computation*, **2013**, 9, 1592-9	6.4	11
127	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
126	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	3.9	11
125	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	3.9	17
124	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, 9141-51	3.4	42
123	Benchmark Values: Thermochemistry of the Ionic Liquid [C4Py][Cl]. *Australian Journal of Chemistry*, **2012**, 65, 1487	1.2	15
122	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
121	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
120	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
119	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
118	Critical behaviour and vapour-liquid coexistence of 1-alkyl-3-methylimidazolium bis(trifluoromethylsulfonyl)amide ionic liquids via Monte Carlo simulations. *Faraday Discussions*, **2012**, 154, 53-69; discussion 81-96, 465-71	3.6	50
117	A comparison of methods for melting point calculation using molecular dynamics simulations. *Journal of Chemical Physics*, **2012**, 136, 144116	3.9	94
116	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
115	An MD study of the applicability of the Walden rule and the Nernst-Einstein model for ionic liquids. *ChemPhysChem*, **2012**, 13, 1701-7	3.2	24
114	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	3.9	63
113	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

112	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
111	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
110	Vapor–liquid Coexistence and Critical Behavior of Ionic Liquids via Molecular Simulations. *Journal of Physical Chemistry Letters*, **2011**, 2, 1439-1443	6.4	65
109	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
108	Reaction Ensemble Monte Carlo Simulation of Complex Molecular Systems. *Journal of Chemical Theory and Computation*, **2011**, 7, 269-79	6.4	31
107	Structure and Dynamics of Neat and CO2-Reacted Ionic Liquid Tetrabutylphosphonium 2-Cyanopyrrolide. *Industrial & Engineering Chemistry Research*, **2011**, 50, 8983-8993	3.9	52
106	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
105	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
104	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
103	Limitations and recommendations for the calculation of shear viscosity using reverse nonequilibrium molecular dynamics. *Journal of Chemical Physics*, **2010**, 132, 014103	3.9	53
102	Historical Perspective and Current Outlook for Molecular Dynamics As a Chemical Engineering Tool. *Industrial & Engineering Chemistry Research*, **2010**, 49, 3059-3078	3.9	86
101	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
100	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
99	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
98	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
97	Molecular Simulation of Polyelectrolye Conformational Dynamics under an AC Electric Field. *Macromolecules*, **2010**, 43, 4805-4813	5.5	18
96	Molecular Simulation of the Thermal and Transport Properties of Three Alkali Nitrate Salts. *Industrial & Engineering Chemistry Research*, **2010**, 49, 559-571	3.9	53
95	What to Do with CO2. *Journal of Physical Chemistry Letters*, **2010**, 1, 3478-3479	6.4	82

94	Molecular dynamics investigation of biomimetic ionic liquids. *Fluid Phase Equilibria*, **2010**, 294, 197-205	2.5	23
93	Atomistic Simulation of Ionic Liquids. *Reviews in Computational Chemistry*, **2009**, 421-493		5
92	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
91	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
90	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
89	COSMO-RS Calculations of Partition Coefficients: Different Tools for Conformation Search. *Chemical Engineering and Technology*, **2009**, 32, 977-986	2	43
88	Molecular simulation of ionic liquids: current status and future opportunities. *Journal of Physics Condensed Matter*, **2009**, 21, 373101	1.8	250
87	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
86	Nanoscale design to enable the revolution in renewable energy. *Energy and Environmental Science*, **2009**, 2, 559	35.4	311
85	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
84	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
83	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
82	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
81	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
80	Ion-Exchange Behavior of One-Dimensional Linked Dodecaniobate Keggin Ion Materials. *Chemistry of Materials*, **2008**, 20, 2513-2521	9.6	50
79	An Atomistic Simulation Study of the Role of Asperities and Indentations on Heterogeneous Bubble Nucleation. *Journal of Heat Transfer*, **2008**, 130,	1.8	20
78	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
77	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

76	Atomistic simulation of water adsorption and cation siting in polyoxoniobate materials. *Microporous and Mesoporous Materials*, **2008**, 116, 532-539	5.3	3
75	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
74	Experimental and theoretical methods to investigate extraframework species in a layered material of dodecaniobate anions. *Inorganic Chemistry*, **2007**, 46, 2067-79	5.1	43
73	Transferable Force Field for Water Adsorption in Cation-Exchanged Titanosilicates. *Industrial & Engineering Chemistry Research*, **2007**, 46, 5754-5765	3.9	3
72	Atomistic simulation of the thermodynamic and transport properties of ionic liquids. *Accounts of Chemical Research*, **2007**, 40, 1200-7	24.3	204
71	Molecular Simulation of Mixtures Containing Imidazolium- and Pyridinium-Based Ionic Liquids and 1-Butanol. *ACS Symposium Series*, **2007**, 102-125	0.4	2
70	Prediction of viscosities and vapor□liquid equilibria for five polyhydric alcohols by molecular simulation. *Fluid Phase Equilibria*, **2007**, 260, 218-231	2.5	58
69	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
68	Comparison of heterogeneous and homogeneous bubble nucleation using molecular simulations. *Physical Review B*, **2007**, 75,	3.3	49
67	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
66	Photoelectron spectrum of isolated ion-pairs in ionic liquid vapor. *Journal of Physical Chemistry A*, **2007**, 111, 3191-5	2.8	98
65	Calculating the enthalpy of vaporization for ionic liquid clusters. *Journal of Physical Chemistry B*, **2007**, 111, 9424-7	3.4	110
64	Isomolar-semigrand ensemble molecular dynamics: application to vapor-liquid equilibrium of the mixture methane/ethane. *Journal of Chemical Physics*, **2006**, 125, 204712	3.9	7
63	Liquid phase behavior of ionic liquids with alcohols: experimental studies and modeling. *Journal of Physical Chemistry B*, **2006**, 110, 9354-61	3.4	127
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