Oleg Borodin

List of Publications by Year
in descending order

267 papers	31,986 citations	4831 · 87 h-index	5102 · 172 g-index
273 all docs	273 docs citations	273 times ranked	19068 citing authors

#	Article	IF	Citations
1	Expanding the low-temperature and high-voltage limits of aqueous lithium-ion battery. Energy Storage Materials, 2022, 45, 903-910.	9.5	58
2	Water/Ionic Liquid/Succinonitrile Hybrid Electrolytes for Aqueous Batteries. Advanced Functional Materials, 2022, 32, .	7.8	11
3	Superionicity in Ionic-Liquid-Based Electrolytes Induced by Positive Ionâ€“Ion Correlations. Journal of the American Chemical Society, 2022, 144, 4657-4666.	6.6	31
4	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
5	Simultaneous Formation of Interphases on both Positive and Negative Electrodes in Highâ€Voltage Aqueous Lithiumâ€Ion Batteries. Small, 2022, 18, e2104986.	5.2	12
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	A sobering examination of the feasibility of aqueous aluminum batteries. Energy and Environmental Science, 2022, 15, 2460-2469.	15.6	27
9	â€œWaterâ€inâ€Eutectogelâ€•Electrolytes for Quasiâ€Solidâ€State Aqueous Lithiumâ€Ion Batteries. Advanced Energy Materials, 2022, 12, .	10.2	27
10	Electrolyte Solvation and Ionic Association: VIII. Reassessing Raman Spectroscopic Studies of Ion Coordination for LiTFSI. Journal of the Electrochemical Society, 2022, 169, 060515.	1.3	13
11	Fire-extinguishing, recyclable liquefied gas electrolytes for temperature-resilient lithium-metal batteries. Nature Energy, 2022, 7, 548-559.	19.8	60
12	Highly reversible Zn metal anode enabled by sustainable hydroxyl chemistry. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	3.3	41
13	Fast Interfacial Kinetics for Multivalent Metal Batteries Enabled By Solvation Sheath Reorganization. ECS Meeting Abstracts, 2022, MA2022-01, 123-123.	0.0	0
14	Identification of LiH and nanocrystalline LiF in the solidâ€“electrolyte interphase of lithium metal anodes. Nature Nanotechnology, 2021, 16, 549-554.	15.6	171
15	Water Domain Enabled Transport in Polymer Electrolytes for Lithium-Ion Batteries. Macromolecules, 2021, 54, 2882-2891.	2.2	6
16	Functionalized Phosphonium Cations Enable Zinc Metal Reversibility in Aqueous Electrolytes. Angewandte Chemie - International Edition, 2021, 60, 12438-12445.	7.2	69
17	Functionalized Phosphonium Cations Enable Zinc Metal Reversibility in Aqueous Electrolytes. Angewandte Chemie, 2021, 133, 12546-12553.	1.6	11
18	A Safer, Wide-Temperature Liquefied Gas Electrolyte Based on Difluoromethane. Journal of Power Sources, 2021, 493, 229668.	4.0	18

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19	(Invited) Electrolyte Design for Alloys Anodes. ECS Meeting Abstracts, 2021, MA2021-01, 116-116.	0.0	0
20	(Invited) Molecular Modeling of Lithium and Zinc Electrolytes. ECS Meeting Abstracts, 2021, MA2021-01, 466-466.	0.0	0
21	Fluorinated interphase enables reversible aqueous zinc battery chemistries. Nature Nanotechnology, 2021, 16, 902-910.	15.6	560
22	Stabilizing the Solidâ€Electrolyte Interphase with Polyacrylamide for Highâ€Voltage Aqueous Lithiumâ€Ion Batteries. Angewandte Chemie - International Edition, 2021, 60, 22812-22817.	7.2	30
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	Minimizing Long-Chain Polysulfide Formation in Li-S Batteries by Using Localized Low Concentration Highly Fluorinated Electrolytes. Journal of the Electrochemical Society, 2021, 168, 090543.	1.3	8
25	Toward Unraveling the Origin of Lithium Fluoride in the Solid Electrolyte Interphase. Chemistry of Materials, 2021, 33, 7315-7336.	3.2	39
26	Stabilizing the Solidâ€Electrolyte Interphase with Polyacrylamide for Highâ€Voltage Aqueous Lithiumâ€Ion Batteries. Angewandte Chemie, 2021, 133, 22994.	1.6	2
27	Solvation sheath reorganization enables divalent metal batteries with fast interfacial charge transfer kinetics. Science, 2021, 374, 172-178.	6.0	238
28	Functionalized Phosphonium Cations Enable Zn Metal Reversibility in Aqueous Electrolytes. ECS Meeting Abstracts, 2021, MA2021-02, 14-14.	0.0	0
29	High-Efficiency Zinc-Metal Anode Enabled by Liquefied Gas Electrolytes. ACS Energy Letters, 2021, 6, 4426-4430.	8.8	21
30	(Battery Division Postdoctoral Associate Research Award Address Sponsored by MTI Corporation and) Tj ETQq0 0 0 rgBT /Overlock 10 Tf Electrochemical Interphases and Enable Highly Reversible Zn Anode. ECS Meeting Abstracts, 2021, MA2021-02, 188-188.	0.0	0
31	Water Domain Enabled Transport and Enhanced Stability in Aqueous Solid Polymer-in-Salt Electrolytes for Lithium-Ion Batteries. ECS Meeting Abstracts, 2021, MA2021-02, 265-265.	0.0	0
32	Improving Electrochemical Stability and Lowâ€Temperature Performance with Water/Acetonitrile Hybrid Electrolytes. Advanced Energy Materials, 2020, 10, 1902654.	10.2	144
33	Highâ€Voltage Aqueous Naâ€Ion Battery Enabled by Inertâ€Cationâ€Assisted Waterâ€inâ€Salt Electrolyte. Advanced Materials, 2020, 32, e1904427.	11.1	221
34	Electrolyte Solvation and Ionic Association. VII. Correlating Raman Spectroscopic Data with Solvate Species. Journal of the Electrochemical Society, 2020, 167, 110551.	1.3	16
35	Realizing high zinc reversibility in rechargeable batteries. Nature Energy, 2020, 5, 743-749.	19.8	658
36	Nanoscale Relaxation in â€œWater-in-Saltâ€ and â€œWater-in-Bisaltâ€ Electrolytes. Journal of Physical Chemistry Letters, 2020, 11, 7279-7284.	2.1	16

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37	Interfacial Speciation Determines Interfacial Chemistry: Xâ€rayâ€Induced Lithium Fluoride Formation from Waterâ€inâ€salt Electrolytes on Solid Surfaces. Angewandte Chemie - International Edition, 2020, 59, 23180-23187.	7.2	28
38	Interfacial Speciation Determines Interfacial Chemistry: Xâ€rayâ€Induced Lithium Fluoride Formation from Waterâ€inâ€salt Electrolytes on Solid Surfaces. Angewandte Chemie, 2020, 132, 23380-23387.	1.6	9
39	Concentration and velocity profiles in a polymeric lithium-ion battery electrolyte. Energy and Environmental Science, 2020, 13, 4312-4321.	15.6	43
40	Boosting High-Performance in Lithiumâ€“Sulfur Batteries via Dilute Electrolyte. Nano Letters, 2020, 20, 5391-5399.	4.5	93
41	Liquefied gas electrolytes for wide-temperature lithium metal batteries. Energy and Environmental Science, 2020, 13, 2209-2219.	15.6	120
42	Critical Factors Dictating Reversibility of the Zinc Metal Anode. Energy and Environmental Materials, 2020, 3, 516-521.	7.3	110
43	A 63 <i>m</i> Superconcentrated Aqueous Electrolyte for High-Energy Li-Ion Batteries. ACS Energy Letters, 2020, 5, 968-974.	8.8	197
44	Uncharted Waters: Super-Concentrated Electrolytes. Joule, 2020, 4, 69-100.	11.7	305
45	Understanding Liâ€Ion Dynamics in Lithium Hydroxychloride (Li 2 OHCl) Solid State Electrolyte via Addressing the Role of Protons. Advanced Energy Materials, 2020, 10, 1903480.	10.2	29
46	Real-time mass spectrometric characterization of the solidâ€“electrolyte interphase of a lithium-ion battery. Nature Nanotechnology, 2020, 15, 224-230.	15.6	280
47	Altering the Electrochemical Pathway of Sulfur Chemistry with Oxygen for High Energy Density and Low Shuttling in a Na/S Battery. ACS Energy Letters, 2020, 5, 1070-1076.	8.8	22
48	Nonflammable Lithium Metal Full Cells with Ultra-high Energy Density Based on Coordinated Carbonate Electrolytes. IScience, 2020, 23, 100844.	1.9	58
49	Electrolyte design for Li metal-free Li batteries. Materials Today, 2020, 39, 118-126.	8.3	138
50	Electrolyte design for LiF-rich solidâ€“electrolyte interfaces to enable high-performance microsized alloy anodes for batteries. Nature Energy, 2020, 5, 386-397.	19.8	621
51	Methyl-group functionalization of pyrazole-based additives for advanced lithium ion battery electrolytes. Journal of Power Sources, 2020, 461, 228159.	4.0	10
52	Liquefied Gas Electrolytes for All-Temperature Lithium Metal Batteries. ECS Meeting Abstracts, 2020, MA2020-01, 373-373.	0.0	0
53	Nucleation, Growth, and Properties of the Solid Electrolyte Interphase â€“ a Multimodal Approach Using a Model System. ECS Meeting Abstracts, 2020, MA2020-02, 860-860.	0.0	0
54	Interfacial Evolution of Layered Oxides in Li-Ion Batteries: Chemical Transformation of Thin-Film Cathodes. ECS Meeting Abstracts, 2020, MA2020-02, 661-661.	0.0	0

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55	(Invited) Electrolyte Design for Li Batteries. ECS Meeting Abstracts, 2020, MA2020-02, 17-17.	0.0	0
56	Critical Factors Dictating Reversibility of the Zinc Metal Anode. ECS Meeting Abstracts, 2020, MA2020-02, 672-672.	0.0	0
57	Potential Dependent Ion Arrangement Near the Electrode/Electrolyte Interface. ECS Meeting Abstracts, 2020, MA2020-02, 719-719.	0.0	0
58	(Invited) Insight into Aqueous and Non-Aqueous Electrolyte Structure, Transport and Interfacial Properties from Molecular Modeling. ECS Meeting Abstracts, 2020, MA2020-02, 744-744.	0.0	0
59	Concentration and Velocity Profiles in a Polymeric Lithium-Ion Battery Electrolyte. ECS Meeting Abstracts, 2020, MA2020-02, 839-839.	0.0	0
60	Identifying the components of the solidâ€“electrolyte interphase in Li-ion batteries. Nature Chemistry, 2019, 11, 789-796.	6.6	331
61	High-Efficiency Lithium-Metal Anode Enabled by Liquefied Gas Electrolytes. Joule, 2019, 3, 2050-2052.	11.7	2
62	High-Efficiency Lithium-Metal Anode Enabled by Liquefied Gas Electrolytes. Joule, 2019, 3, 1986-2000.	11.7	183
63	A Pyrazineâ€Based Polymer for Fastâ€Charge Batteries. Angewandte Chemie - International Edition, 2019, 58, 17820-17826.	7.2	173
64	A Pyrazineâ€Based Polymer for Fastâ€Charge Batteries. Angewandte Chemie, 2019, 131, 17984-17990.	1.6	19
65	Transport Properties of Li-TFSI Water-in-Salt Electrolytes. Journal of Physical Chemistry B, 2019, 123, 10514-10521.	1.2	60
66	Bisalt ether electrolytes: a pathway towards lithium metal batteries with Ni-rich cathodes. Energy and Environmental Science, 2019, 12, 780-794.	15.6	310
67	Molecular Dynamics Simulations of Ionic Liquids and Electrolytes Using Polarizable Force Fields. Chemical Reviews, 2019, 119, 7940-7995.	23.0	386
68	Probing Electric Double-Layer Composition via in Situ Vibrational Spectroscopy and Molecular Simulations. Journal of Physical Chemistry Letters, 2019, 10, 3381-3389.	2.1	27
69	Aqueous Li-ion battery enabled by halogen conversionâ€“intercalation chemistry in graphite. Nature, 2019, 569, 245-250.	13.7	590
70	Challenges with prediction of battery electrolyte electrochemical stability window and guiding the electrode â€“ electrolyte stabilization. Current Opinion in Electrochemistry, 2019, 13, 86-93.	2.5	72
71	Fading Mechanisms and Voltage Hysteresis in FeF₂â€“NiF₂ Solid Solution Cathodes for Lithium and Lithiumâ€Ion Batteries. Small, 2019, 15, e1804670.	5.2	62
72	(Invited) Molecular Scale Modeling of Structure, Transport and Electrochemistry of Aqueous and Non-Aqueous Electrolytes. ECS Meeting Abstracts, 2019, , .	0.0	0

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73	Sulfone-Based Electrolytes for Next Generation Lithium Batteries. ECS Meeting Abstracts, 2019, , .	0.0	0
74	Layered LiTiO₂ for the protection of Li₂S cathodes against dissolution: mechanisms of the remarkable performance boost. Energy and Environmental Science, 2018, 11, 807-817.	15.6	103
75	A carbonate-free, sulfone-based electrolyte for high-voltage Li-ion batteries. Materials Today, 2018, 21, 341-353.	8.3	258
76	Highly reversible zinc metal anode for aqueous batteries. Nature Materials, 2018, 17, 543-549.	13.3	2,080
77	Investigation of Ionâ€“Solvent Interactions in Nonaqueous Electrolytes Using in Situ Liquid SIMS. Analytical Chemistry, 2018, 90, 3341-3348.	3.2	41
78	Azo compounds as a family of organic electrode materials for alkali-ion batteries. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 2004-2009.	3.3	168
79	The nanoscale structure of the electrolyteâ€“metal oxide interface. Energy and Environmental Science, 2018, 11, 594-602.	15.6	46
80	Application of Screening Functions as Cutoff-Based Alternatives to Ewald Summation in Molecular Dynamics Simulations Using Polarizable Force Fields. Journal of Chemical Theory and Computation, 2018, 14, 768-783.	2.3	7
81	Hybrid Aqueous/Non-aqueous Electrolyte for Safe and High-Energy Li-Ion Batteries. Joule, 2018, 2, 927-937.	11.7	303
82	Protons Enhance Conductivities in Lithium Halide Hydroxide/Lithium Oxyhalide Solid Electrolytes by Forming Rotating Hydroxy Groups. Advanced Energy Materials, 2018, 8, 1700971.	10.2	65
83	Hybrid Aqueous/Non-aqueous Electrolyte for Safe and High-Energy Li-Ion Batteries. Joule, 2018, 2, 2178.	11.7	12
84	Cation-Dependent Electrochemistry of Polysulfides in Lithium and Magnesium Electrolyte Solutions. Journal of Physical Chemistry C, 2018, 122, 21770-21783.	1.5	49
85	Multinuclear magnetic resonance investigation of cation-anion and anion-solvent interactions in carbonate electrolytes. Journal of Power Sources, 2018, 399, 215-222.	4.0	19
86	Non-flammable electrolyte enables Li-metal batteries with aggressive cathode chemistries. Nature Nanotechnology, 2018, 13, 715-722.	15.6	964
87	Lithiumâ€“Iron (III) Fluoride Battery with Double Surface Protection. Advanced Energy Materials, 2018, 8, 1800721.	10.2	67
88	Insights into the Structure and Transport of the Lithium, Sodium, Magnesium, and Zinc Bis(trifluoromethansulfonyl)imide Salts in Ionic Liquids. Journal of Physical Chemistry C, 2018, 122, 20108-20121.	1.5	64
89	Fundamental Investigations into Na+ Behavior in Aqueous and Non-Aqueous Electrolytes. ECS Meeting Abstracts, 2018, , .	0.0	0
90	(Invited) Recent Progress in Understanding Battery Electrolyte Electrochemical Stability and Its Relationship with Electrolyte Structural Properties. ECS Meeting Abstracts, 2018, , .	0.0	0

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91	Relaxation in a Prototype Ionic Liquid: Influence of Water on the Dynamics. Journal of Physical Chemistry Letters, 2017, 8, 715-719.	2.1	11
92	Formation of Reversible Solid Electrolyte Interface on Graphite Surface from Concentrated Electrolytes. Nano Letters, 2017, 17, 1602-1609.	4.5	91
93	On the application of constant electrode potential simulation techniques in atomistic modelling of electric double layers. Molecular Simulation, 2017, 43, 838-849.	0.9	34
94	Solvation behavior of carbonate-based electrolytes in sodium ion batteries. Physical Chemistry Chemical Physics, 2017, 19, 574-586.	1.3	152
95	Unique aqueous Li-ion/sulfur chemistry with high energy density and reversibility. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 6197-6202.	3.3	151
96	Spectroscopic and Density Functional Theory Characterization of Common Lithium Salt Solvates in Carbonate Electrolytes for Lithium Batteries. Journal of Physical Chemistry C, 2017, 121, 2135-2148.	1.5	114
97	Liquid Structure with Nano-Heterogeneity Promotes Cationic Transport in Concentrated Electrolytes. ACS Nano, 2017, 11, 10462-10471.	7.3	283
98	Ramifications of Water-in-Salt Interfacial Structure at Charged Electrodes for Electrolyte Electrochemical Stability. Journal of Physical Chemistry Letters, 2017, 8, 4362-4367.	2.1	150
99	Charge storage at the nanoscale: understanding the trends from the molecular scale perspective. Journal of Materials Chemistry A, 2017, 5, 21049-21076.	5.2	58
100	4.0ÂV Aqueous Li-Ion Batteries. Joule, 2017, 1, 122-132.	11.7	441
101	â€œWaterâ€inâ€Saltâ€•Electrolyte Makes Aqueous Sodiumâ€Ion Battery Safe, Green, and Longâ€Lasting. Advanced Energy Materials, 2017, 7, 1701189.	10.2	487
102	In situ surface protection for enhancing stability and performance of conversion-type cathodes. MRS Energy & Sustainability, 2017, 4, 1.	1.3	47
103	Toward in-situ protected sulfur cathodes by using lithium bromide and pre-charge. Nano Energy, 2017, 40, 170-179.	8.2	53
104	How Solid-Electrolyte Interphase Forms in Aqueous Electrolytes. Journal of the American Chemical Society, 2017, 139, 18670-18680.	6.6	365
105	Modeling Insight into Battery Electrolyte Electrochemical Stability and Interfacial Structure. Accounts of Chemical Research, 2017, 50, 2886-2894.	7.6	234
106	Li⁺ Transport and Mechanical Properties of Model Solid Electrolyte Interphases (SEI): Insight from Atomistic Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2017, 121, 16098-16109.	1.5	76
107	Insight into Structure and Transport of the Lithium, Sodium, Magnesium and Zinc Bis(trifluoromethansulfonyl)Imide Salts in Ionic Liquids. ECS Meeting Abstracts, 2017, , .	0.0	0
108	Influence of Protons on the Lithium Transport Mechanism in Antiperovskite Solid Electrolytes from Molecular Dynamics Simulations. ECS Meeting Abstracts, 2017, , .	0.0	0

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109	Structure and Transport of â€œWater-in-Saltâ€• Electrolytes from Molecular Dynamics Simulations. ECS Meeting Abstracts, 2017, , .	0.0	1
110	Renewed Interest in Sulfone-Based Electrolytes for 5V Li-Ion Batteries. ECS Meeting Abstracts, 2017, , .	0.0	0
111	Computational and Spectroscopic Analysis of Ion Interactions in Sodium and Lithium Ion Battery Electrolytes. ECS Meeting Abstracts, 2017, , .	0.0	0
112	A Molecular Dynamics Study of Concentrated Aqueous Solutions of Lithium Salts at Charged Electrodes. ECS Meeting Abstracts, 2017, , .	0.0	0
113	(Invited) Liquid and Solid State NMR Investigations of Electrolytes for Beyond Lithium Ion Applications. ECS Meeting Abstracts, 2017, , .	0.0	0
114	Advanced Highâ€Voltage Aqueous Lithiumâ€Ion Battery Enabled by â€œWaterâ€inâ€Bisaltâ€• Electrolyte. Angewandte Chemie, 2016, 128, 7252-7257.	1.6	459
115	cDPD: A new dissipative particle dynamics method for modeling electrokinetic phenomena at the mesoscale. Journal of Chemical Physics, 2016, 145, 144109.	1.2	20
116	Sensitivity of Density Functional Theory Methodology for Oxygen Reduction Reaction Predictions on Feâ€“N₄-Containing Graphitic Clusters. Journal of Physical Chemistry C, 2016, 120, 28545-28562.	1.5	31
117	Effect of water on the structure of a prototype ionic liquid. Physical Chemistry Chemical Physics, 2016, 18, 23474-23481.	1.3	23
118	Importance of Reduction and Oxidation Stability of High Voltage Electrolytes and Additives. Electrochimica Acta, 2016, 209, 498-510.	2.6	179
119	Conversion Cathodes: Lithiumâ€“Iron Fluoride Battery with In Situ Surface Protection (Adv. Funct.) Tj ETQq1 1 0.784314 rgBT /Overlock	7.8	1
120	Computer Simulations of Ion Transport in Polymer Electrolyte Membranes. Annual Review of Chemical and Biomolecular Engineering, 2016, 7, 349-371.	3.3	84
121	A comparative study of room temperature ionic liquids and their organic solvent mixtures near charged electrodes. Journal of Physics Condensed Matter, 2016, 28, 464002.	0.7	30
122	Lithiumâ€“Iron Fluoride Battery with In Situ Surface Protection. Advanced Functional Materials, 2016, 26, 1507-1516.	7.8	73
123	Activation of Oxygenâ€Stabilized Sulfur for Li and Na Batteries. Advanced Functional Materials, 2016, 26, 745-752.	7.8	80
124	Advanced Highâ€Voltage Aqueous Lithiumâ€Ion Battery Enabled by â€œWaterâ€inâ€Bisaltâ€• Electrolyte. Angewandte Chemie - International Edition, 2016, 55, 7136-7141.	7.2	571
125	Competitive lithium solvation of linear and cyclic carbonates from quantum chemistry. Physical Chemistry Chemical Physics, 2016, 18, 164-175.	1.3	165
126	Importance of Ion Packing on the Dynamics of Ionic Liquids during Micropore Charging. Journal of Physical Chemistry Letters, 2016, 7, 36-42.	2.1	78

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127	Natural abundance 17O, 6Li NMR and molecular modeling studies of the solvation structures of lithium bis(fluorosulfonyl)imide/1,2-dimethoxyethane liquid electrolytes. Journal of Power Sources, 2016, 307, 231-243.	4.0	58
128	The influence of cations on lithium ion coordination and transport in ionic liquid electrolytes: a MD simulation study. Physical Chemistry Chemical Physics, 2016, 18, 382-392.	1.3	59
129	Anion Solvation in Carbonate-Based Electrolytes. Journal of Physical Chemistry C, 2015, 119, 27255-27264.	1.5	121
130	Effect of Organic Solvents on Li⁺ Ion Solvation and Transport in Ionic Liquid Electrolytes: A Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2015, 119, 3085-3096.	1.2	78
131	Electrolyte Solvation and Ionic Association. Journal of the Electrochemical Society, 2015, 162, A501-A510.	1.3	32
132	<i>Ab Initio</i> Characterization of the Electrochemical Stability and Solvation Properties of Condensed-Phase Ethylene Carbonate and Dimethyl Carbonate Mixtures. Journal of Physical Chemistry C, 2015, 119, 3865-3880.	1.5	50
133	High rate and stable cycling of lithium metal anode. Nature Communications, 2015, 6, 6362.	5.8	1,954
134	Solvate Structures and Computational/Spectroscopic Characterization of LiPF₆ Electrolytes. Journal of Physical Chemistry C, 2015, 119, 8492-8500.	1.5	79
135	Quantification of sampling uncertainty for molecular dynamics simulation: Time-dependent diffusion coefficient in simple fluids. Journal of Computational Physics, 2015, 302, 485-508.	1.9	29
136	Towards high throughput screening of electrochemical stability of battery electrolytes. Nanotechnology, 2015, 26, 354003.	1.3	160
137	â€œWater-in-saltâ€• electrolyte enables high-voltage aqueous lithium-ion chemistries. Science, 2015, 350, 938-943.	6.0	2,553
138	ReaxFF molecular dynamics simulations on lithiated sulfur cathode materials. Physical Chemistry Chemical Physics, 2015, 17, 3383-3393.	1.3	143
139	In Situ Formation of Protective Coatings on Sulfur Cathodes in Lithium Batteries with LiFSIâ€Based Organic Electrolytes. Advanced Energy Materials, 2015, 5, 1401792.	10.2	189
140	Lithium Iodide as a Promising Electrolyte Additive for Lithiumâ€“Sulfur Batteries: Mechanisms of Performance Enhancement. Advanced Materials, 2015, 27, 101-108.	11.1	304
141	Electrolyte Solvation and Ionic Association. Journal of the Electrochemical Society, 2014, 161, A2042-A2053.	1.3	104
142	Molecular Modeling of Electrolytes. Modern Aspects of Electrochemistry, 2014, , 371-401.	0.2	24
143	Solvate Structures and Spectroscopic Characterization of LiTFSI Electrolytes. Journal of Physical Chemistry B, 2014, 118, 13601-13608.	1.2	121
144	Concentrated electrolytes: decrypting electrolyte properties and reassessing Al corrosion mechanisms. Energy and Environmental Science, 2014, 7, 416-426.	15.6	332

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145	Quantum chemistry study of the oxidation-induced stability and decomposition of propylene carbonate-containing complexes. Physical Chemistry Chemical Physics, 2014, 16, 6560.	1.3	33
146	X-Ray absorption spectroscopy of LiBF₄ in propylene carbonate: a model lithium ion battery electrolyte. Physical Chemistry Chemical Physics, 2014, 16, 23568-23575.	1.3	46
147	Correction to â€œMolecular Dynamics Simulation Study of the Interfacial Structure and Differential Capacitance of Alkylimidazolium Bis(trifluoromethanesulfonyl)imide [C_{<i>n</i>}mim][TFSI] Ionic Liquids at Graphite Electrodesâ€ Journal of Physical Chemistry C, 2014, 118, 18283-18283.	1.5	0
148	Interfacial Structure and Dynamics of the Lithium Alkyl Dicarbonate SEI Components in Contact with the Lithium Battery Electrolyte. Journal of Physical Chemistry C, 2014, 118, 18362-18371.	1.5	71
149	The Effect of Low-Molecular-Weight Poly(ethylene glycol) (PEG) Plasticizers on the Transport Properties of Lithium Fluorosulfonimide Ionic Melt Electrolytes. Journal of Physical Chemistry B, 2014, 118, 5135-5143.	1.2	19
150	Structure and Energetics of Li⁺â€“(BF₄^{â€“})_{<i>n</i>}, Li⁺â€“(FSI^{â€“})_{<i>n</i>}, and Li⁺â€“(TFSI^{â€“})_{<i>n</i>}: Ab Initio and Polarizable Force Field Approaches. Journal of Physical Chemistry B, 2014, 118, 10785-10794.	1.2	31
151	A comparative study of alkylimidazolium room temperature ionic liquids with FSI and TFSI anions near charged electrodes. Electrochimica Acta, 2014, 145, 40-52.	2.6	52
152	A Combined Theoretical and Experimental Study of the Influence of Different Anion Ratios on Lithium Ion Dynamics in Ionic Liquids. Journal of Physical Chemistry B, 2014, 118, 7367-7375.	1.2	88
153	Computational and Experimental Investigation of Li-Doped Ionic Liquid Electrolytes: [pyr14][TFSI], [pyr13][FSI], and [EMIM][BF₄]. Journal of Physical Chemistry B, 2014, 118, 11295-11309.	1.2	131
154	Combined quantum chemical/Raman spectroscopic analyses of Li+ cation solvation: Cyclic carbonate solventsâ€”Ethylene carbonate and propylene carbonate. Journal of Power Sources, 2014, 267, 821-830.	4.0	71
155	High Voltage Li-Ion Battery Development. ECS Meeting Abstracts, 2014, , .	0.0	0
156	Transport in Concentrated Solutions. , 2014, , 2091-2098.		0
157	Electrolytes for Li-Ion Batteries Based on High Voltage Cathodes. ECS Meeting Abstracts, 2014, , .	0.0	0
158	Oxidative Stability and Initial Decomposition Reactions of Carbonate, Sulfone, and Alkyl Phosphate-Based Electrolytes. Journal of Physical Chemistry C, 2013, 117, 8661-8682.	1.5	283
159	A molecular dynamics simulation study of the electric double layer and capacitance of [BMIM][PF6] and [BMIM][BF4] room temperature ionic liquids near charged surfaces. Physical Chemistry Chemical Physics, 2013, 15, 14234.	1.3	93
160	Electrolyte Solvation and Ionic Association III. Acetonitrile-Lithium Salt Mixturesâ€“Transport Properties. Journal of the Electrochemical Society, 2013, 160, A1061-A1070.	1.3	136
161	Electrolyte Solvation and Ionic Association. Journal of the Electrochemical Society, 2013, 160, A2100-A2110.	1.3	43
162	Physicochemical Properties of Binary Ionic Liquidâ€“Aprotic Solvent Electrolyte Mixtures. Journal of Physical Chemistry C, 2013, 117, 78-84.	1.5	64

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163	On the Atomistic Nature of Capacitance Enhancement Generated by Ionic Liquid Electrolyte Confined in Subnanometer Pores. Journal of Physical Chemistry Letters, 2013, 4, 132-140.	2.1	107
164	Lithium Battery Electrolyte Stability and Performance from Molecular Modeling and Simulations. , 2013, , 195-237.		1
165	Molecular Dynamics Simulations and Experimental Study of Lithium Ion Transport in Dilithium Ethylene Dicarbonate. Journal of Physical Chemistry C, 2013, 117, 7433-7444.	1.5	92
166	Influence of Solvent on Ion Aggregation and Transport in PY₁₅TFSI Ionic Liquidâ€“Aprotic Solvent Mixtures. Journal of Physical Chemistry B, 2013, 117, 10581-10588.	1.2	35
167	Quantum Chemistry Study of the Oxidation-Induced Decomposition of Tetramethylene Sulfone (TMS) Dimer and TMS/BF₄ ⁻. ECS Transactions, 2013, 50, 391-398.	0.3	8
168	Molecular dynamics simulation studies of the influence of imidazolium structure on the properties of imidazolium/azide ionic liquids. Journal of Chemical Physics, 2012, 136, 194506.	1.2	16
169	Molecular Dynamics Simulation Study of the Interfacial Structure and Differential Capacitance of Alkylimidazolium Bis(trifluoromethanesulfonyl)imide [C_{<i>n</i>}mim][TFSI] Ionic Liquids at Graphite Electrodes. Journal of Physical Chemistry C, 2012, 116, 7940-7951.	1.5	144
170	Li+ cation coordination by acetonitrileâ€”insights from crystallography. RSC Advances, 2012, 2, 8014.	1.7	39
171	Electrolyte Solvation and Ionic Association. Journal of the Electrochemical Society, 2012, 159, A553-A565.	1.3	170
172	Electrolyte Solvation and Ionic Association II. Acetonitrile-Lithium Salt Mixtures: Highly Dissociated Salts. Journal of the Electrochemical Society, 2012, 159, A1489-A1500.	1.3	269
173	Correlating Li⁺ Solvation Sheath Structure with Interphasial Chemistry on Graphite. Journal of Physical Chemistry C, 2012, 116, 26111-26117.	1.5	166
174	Electrode/Electrolyte Interface in Sulfolane-Based Electrolytes for Li Ion Batteries: A Molecular Dynamics Simulation Study. Journal of Physical Chemistry C, 2012, 116, 23871-23881.	1.5	126
175	Molecular Dynamics Simulation Studies of the Structure of a Mixed Carbonate/LiPF₆ Electrolyte near Graphite Surface as a Function of Electrode Potential. Journal of Physical Chemistry C, 2012, 116, 1114-1121.	1.5	191
176	Oxidation induced decomposition of ethylene carbonate from DFT calculations â€“ importance of explicitly treating surrounding solvent. Physical Chemistry Chemical Physics, 2012, 14, 12838.	1.3	133
177	Insight into Electrolyte Stability, Decomposition and Transport Properties from DFT and MD Simulations. ECS Meeting Abstracts, 2012, , .	0.0	0
178	Quantum Chemistry Studies of the Oxidative Stability of Carbonate, Sulfone and Sulfonate-Based Electrolytes Doped with BF₄ ⁻, PF₆ ⁻ Anions. ECS Transactions, 2011, 33, 77-84.	0.3	63
179	Development of a Polarizable Force Field for Molecular Dynamics Simulations of Poly (Ethylene) Tj ETQq1 1 0.784314 rgBT /Overlock	2.3	39
180	Insight into Hydrazinium Nitrates, Azides, Dicyanamide, and 5-Azidotetrazolate Ionic Materials from Simulations and Experiments. Journal of Physical Chemistry B, 2011, 115, 13578-13592.	1.2	10

#	Article	IF	Citations
181	Molecular Simulations of the Electric Double Layer Structure, Differential Capacitance, and Charging Kinetics for <i>N</i>-Methyl-<i>N</i>-propylpyrrolidinium Bis(fluorosulfonyl)imide at Graphite Electrodes. Journal of Physical Chemistry B, 2011, 115, 3073-3084.	1.2	164
182	On the Influence of Surface Topography on the Electric Double Layer Structure and Differential Capacitance of Graphite/Ionic Liquid Interfaces. Journal of Physical Chemistry Letters, 2011, 2, 2267-2272.	2.1	152
183	Density Functional Theory Study of the Role of Anions on the Oxidative Decomposition Reaction of Propylene Carbonate. Journal of Physical Chemistry A, 2011, 115, 13896-13905.	1.1	184
184	(Invited) Bulk and Interfacial Behavior of Ionic Liquids from Molecular Dynamics Simulations. ECS Transactions, 2010, 33, 583-599.	0.3	4
185	Mechanical and Dynamic Properties of N,N,N,N-Tetramethylammonium Dicyanamide Plastic Crystal. ECS Transactions, 2010, 33, 641-657.	0.3	2
186	Molecular Insights into the Potential and Temperature Dependences of the Differential Capacitance of a Room-Temperature Ionic Liquid at Graphite Electrodes. Journal of the American Chemical Society, 2010, 132, 14825-14833.	6.6	297
187	Thermodynamic, Dynamic, and Structural Properties of Ionic Liquids Comprised of 1-Butyl-3-methylimidazolium Cation and Nitrate, Azide, or Dicyanamide Anions. Journal of Physical Chemistry B, 2010, 114, 12802-12810.	1.2	34
188	Influence of Polarization on Structural, Thermodynamic, and Dynamic Properties of Ionic Liquids Obtained from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2010, 114, 4984-4997.	1.2	140
189	Understanding the Lithium Transport within a Rouse-Based Model for a PEO/LiTFSI Polymer Electrolyte. Macromolecules, 2010, 43, 2028-2036.	2.2	162
190	Molecular Dynamics Simulation and Pulsed-Field Gradient NMR Studies of Bis(fluorosulfonyl)imide (FSI) and Bis[(trifluoromethyl)sulfonyl]imide (TFSI)-Based Ionic Liquids. Journal of Physical Chemistry B, 2010, 114, 6786-6798.	1.2	190
191	Molecular dynamics simulations of atomically flat and nanoporous electrodes with a molten salt electrolyte. Physical Chemistry Chemical Physics, 2010, 12, 170-182.	1.3	114
192	A comparison of fluoroalkyl-derivatized imidazolium:TFSI and alkyl-derivatized imidazolium:TFSI ionic liquids: a molecular dynamics simulation study. Physical Chemistry Chemical Physics, 2010, 12, 7064.	1.3	48
193	Molecular dynamics simulations of N,N,N,N-tetramethylammonium dicyanamide plastic crystal and liquid using a polarizable force field. Physical Chemistry Chemical Physics, 2010, 12, 4635.	1.3	29
194	A molecular dynamics simulation study of the pressure-volume-temperature behavior of polymers under high pressure. Journal of Chemical Physics, 2009, 130, 144904.	1.2	39
195	Quantum Chemistry and Molecular Dynamics Simulation Study of Dimethyl Carbonate: Ethylene Carbonate Electrolytes Doped with LiPF₆. Journal of Physical Chemistry B, 2009, 113, 1763-1776.	1.2	264
196	A molecular dynamics simulation study of crystalline 1,3,5-triamino-2,4,6-trinitrobenzene as a function of pressure and temperature. Journal of Chemical Physics, 2009, 131, 224703.	1.2	91
197	Effect of Ion Distribution on Conductivity of Block Copolymer Electrolytes. Nano Letters, 2009, 9, 1212-1216.	4.5	228
198	Relation between Heat of Vaporization, Ion Transport, Molar Volume, and Cationâˆ’Anion Binding Energy for Ionic Liquids. Journal of Physical Chemistry B, 2009, 113, 12353-12357.	1.2	88

#	Article	IF	Citations
199	A molecular dynamics simulation study of LiFePO4/electrolyte interfaces: structure and Li+ transport in carbonate and ionic liquid electrolytes. Physical Chemistry Chemical Physics, 2009, 11, 9884.	1.3	55
200	Polarizable Force Field Development and Molecular Dynamics Simulations of Ionic Liquids. Journal of Physical Chemistry B, 2009, 113, 11463-11478.	1.2	581
201	Viscosity of a Room Temperature Ionic Liquid: Predictions from Nonequilibrium and Equilibrium Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2009, 113, 4771-4774.	1.2	81
202	A comparison of ether- and alkyl-derivatized imidazolium-based room-temperature ionic liquids: a molecular dynamics simulation study. Physical Chemistry Chemical Physics, 2008, 10, 6301.	1.3	125
203	Polarizable and Nonpolarizable Force Fields for Alkyl Nitrates. Journal of Physical Chemistry B, 2008, 112, 734-742.	1.2	32
204	Molecular Dynamics Simulations of Ionic Liquids: Influence of Polarization on IL Structure and Ion Transport. Materials Research Society Symposia Proceedings, 2008, 1082, 60401.	0.1	6
205	Interfacial properties of semifluorinated alkane diblock copolymers. Journal of Chemical Physics, 2008, 128, 214903.	1.2	35
206	Molecular Dynamics Simulations of LiFePO4/Electrolyte Interfaces. ECS Meeting Abstracts, 2008, , .	0.0	0
207	Molecular Dynamics Simulations of Comb-Branched Poly(epoxide ether)-Based Polymer Electrolytes. Macromolecules, 2007, 40, 1252-1258.	2.2	41
208	Comment on â€œOn the Accuracy of Force Fields for Predicting the Physical Properties of Dimethylnitramineâ€. Journal of Physical Chemistry B, 2007, 111, 1900-1902.	1.2	13
209	A molecular dynamics simulation and quantum chemistry study of poly(dimethylsiloxane)â€“silica nanoparticle interactions. Journal of Polymer Science, Part B: Polymer Physics, 2007, 45, 1599-1615.	2.4	53
210	Li + Transport Mechanism in Oligo(Ethylene Oxide)s Compared to Carbonates. Journal of Solution Chemistry, 2007, 36, 803-813.	0.6	57
211	Development of Manyâ˘'Body Polarizable Force Fields for Li-Battery Applications:Â 2. LiTFSI-Doped Oligoether, Polyether, and Carbonate-Based Electrolytes. Journal of Physical Chemistry B, 2006, 110, 6293-6299.	1.2	127
212	Li+ Cation Environment, Transport, and Mechanical Properties of the LiTFSI Doped N-Methyl-N-alkylpyrrolidinium+TFSI- Ionic Liquids. Journal of Physical Chemistry B, 2006, 110, 16879-16886.	1.2	303
213	Mechanism of Ion Transport in Amorphous Poly(ethylene oxide)/LiTFSI from Molecular Dynamics Simulations. Macromolecules, 2006, 39, 1620-1629.	2.2	432
214	Structure and Dynamics ofN-Methyl-N-propylpyrrolidinium Bis(trifluoromethanesulfonyl)imide Ionic Liquid from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2006, 110, 11481-11490.	1.2	221
215	Development of Manyâ˘'Body Polarizable Force Fields for Li-Battery Components:Â 1. Ether, Alkane, and Carbonate-Based Solvents. Journal of Physical Chemistry B, 2006, 110, 6279-6292.	1.2	149
216	Li+Transport in Lithium Sulfonylimideâ˘'Oligo(ethylene oxide) Ionic Liquids and Oligo(ethylene oxide) Doped with LiTFSI. Journal of Physical Chemistry B, 2006, 110, 24266-24274.	1.2	57

#	Article	IF	Citations
217	Molecular Dynamics Simulations of Lithium Alkyl Carbonates. Journal of Physical Chemistry B, 2006, 110, 22773-22779.	1.2	97
218	Modeling of enhanced penetrant diffusion in nanoparticle-polymer composite membranes. Journal of Membrane Science, 2006, 286, 293-300.	4.1	27
219	LiTFSI Structure and Transport in Ethylene Carbonate from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2006, 110, 4971-4977.	1.2	170
220	Micromechanics simulations of the viscoelastic properties of highly filled composites by the material point method (MPM). Modelling and Simulation in Materials Science and Engineering, 2006, 14, 703-720.	0.8	13
221	Ion Transport in Single Ion Conductors. ECS Meeting Abstracts, 2006, , .	0.0	0
222	MD Simulations Study of Liquid Electrolytes and SEI Components. ECS Meeting Abstracts, 2006, , .	0.0	0
223	Multiscale modeling of viscoelastic properties of polymer nanocomposites. Journal of Polymer Science, Part B: Polymer Physics, 2005, 43, 1005-1013.	2.4	46
224	Quantum Chemistryâ€"Based Force Field for Simulations of Energetic Dinitro Compounds. Journal of Energetic Materials, 2005, 23, 205-237.	1.0	8
225	Frictional Dynamics of Fluorine-Terminated Alkanethiol Self-Assembled Monolayers. Langmuir, 2004, 20, 10007-10014.	1.6	30
226	Molecular dynamics study of nanocomposite polymer electrolyte based on poly(ethylene oxide)/LiBF4. Modelling and Simulation in Materials Science and Engineering, 2004, 12, S73-S89.	0.8	35
227	A Quantum Chemistry Based Force Field for Poly(dimethylsiloxane). Journal of Physical Chemistry B, 2004, 108, 20340-20350.	1.2	53
228	A Quantum-Chemistry-Based Potential for a Poly(ester urethane). Journal of Physical Chemistry A, 2003, 107, 7552-7560.	1.1	22
229	Transport Properties of Perfluoroalkanes Using Molecular Dynamics Simulation:Â Comparison of United- and Explicit-Atom Models. Industrial & Engineering Chemistry Research, 2003, 42, 6956-6961.	1.8	19
230	MD Simulations and Experimental Study of Structure, Dynamics, and Thermodynamics of Poly(ethylene) Tj ETQq0 0 0 rgBT /Overlock 10	1.2	58
231	Quasielastic Neutron-Scattering Study of the Local Dynamics of Poly(ethylene glycol) Dimethyl Ether in Aqueous Solution. Journal of Physical Chemistry B, 2003, 107, 10446-10452.	1.2	12
232	Development of Quantum Chemistry-Based Force Fields for Poly(ethylene oxide) with Many-Body Polarization Interactions. Journal of Physical Chemistry B, 2003, 107, 6801-6812.	1.2	74
233	Molecular Dynamics Study of the Influence of Solid Interfaces on Poly(ethylene oxide) Structure and Dynamics. Macromolecules, 2003, 36, 7873-7883.	2.2	114
234	Force Field Development and MD Simulations of Poly(ethylene oxide)/LiBF4 Polymer Electrolytes. Journal of Physical Chemistry B, 2003, 107, 6824-6837.	1.2	100

#	Article	IF	Citations
235	Structural Relaxation and Dynamic Heterogeneity in a Polymer Melt at Attractive Surfaces. Physical Review Letters, 2003, 90, 226103.	2.9	82
236	A molecular-dynamics simulation study of dielectric relaxation in a 1,4-polybutadiene melt. Journal of Chemical Physics, 2002, 117, 10350-10359.	1.2	75
237	Microwave Dielectric Relaxation, Electrical Conductance, and Ultrasonic Relaxation of LiPF6 in Poly(ethylene oxide) Dimethyl Ether-500. Journal of Physical Chemistry B, 2002, 106, 2140-2145.	1.2	15
238	Molecular Dynamics Simulation Study of Dielectric Relaxation in Aqueous Poly(ethylene oxide) Solutions. Macromolecules, 2002, 35, 2410-2412.	2.2	28
239	Temperature Dependence of Water Dynamics in Poly(Ethylene Oxide)/Water Solutions from Molecular Dynamics Simulations and Quasielastic Neutron Scattering Experiments. Journal of Physical Chemistry B, 2002, 106, 5184-5193.	1.2	35
240	Concentration Dependence of Water Dynamics in Poly(Ethylene Oxide)/Water Solutions from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2002, 106, 5194-5199.	1.2	45
241	A Quantum Chemistry Based Force Field for Perfluoroalkanes and Poly(tetrafluoroethylene). Journal of Physical Chemistry B, 2002, 106, 9912-9922.	1.2	86
242	A revised quantum chemistry-based potential for poly(ethylene oxide) and its oligomers in aqueous solution. Journal of Computational Chemistry, 2002, 23, 1480-1488.	1.5	72
243	Coherent neutron scattering from PEO and a PEO-based polymer electrolyte. Solid State Ionics, 2002, 147, 225-236.	1.3	39
244	The structure of a poly(ethylene oxide) melt from neutron scattering and molecular dynamics simulations. Journal of Chemical Physics, 2001, 115, 10998-11003.	1.2	31
245	A Molecular Dynamics Simulation Study of Polymer Dynamics in Aqueous Poly(ethylene oxide) Solutions. Macromolecules, 2001, 34, 5687-5693.	2.2	36
246	A Density Functional Theory Study of the Structure and Energetics of Zincate Complexes. Journal of Physical Chemistry A, 2001, 105, 6506-6512.	1.1	29
247	13C NMR Spinâ˘Lattice Relaxation and Conformational Dynamics in a 1,4-Polybutadiene Melt. Macromolecules, 2001, 34, 5192-5199.	2.2	74
248	Dynamic heterogeneity in polymer electrolytes. Comparison between QENS data and MD simulations. Physica B: Condensed Matter, 2001, 301, 163-167.	1.3	33
249	Ab initio quantum chemistry and molecular dynamics simulations studies of LiPF6/poly(ethylene oxide) interactions. Journal of Computational Chemistry, 2001, 22, 641-654.	1.5	76
250	Polarizable and nonpolarizable potentials for K+ cation in water. Chemical Physics Letters, 2001, 336, 292-302.	1.2	26
251	Ab initio quantum chemistry and molecular dynamics simulations studies of LiPF6/poly(ethylene oxide) interactions. Journal of Computational Chemistry, 2001, 22, 641-654.	1.5	3
252	Diffusion in aqueous solutions of 1,2-dimethoxyethane: comparison of molecular dynamics simulations and quasielastic neutron scattering. Chemical Physics, 2000, 261, 137-148.	0.9	7

#	Article	IF	Citations
253	Molecular Dynamics Simulation Study of Hydrogen Bonding in Aqueous Poly(Ethylene Oxide) Solutions. Physical Review Letters, 2000, 85, 5583-5586.	2.9	124
254	Molecular-dynamics simulation of structural and conformational properties of poly(propylene) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 702	1.2	18
255	Molecular Dynamics Simulation Study of LiI-Doped Diglyme and Poly(ethylene oxide) Solutions. Journal of Physical Chemistry B, 2000, 104, 8017-8022.	1.2	32
256	A Study of the Influence of LiI on the Chain Conformations of Poly(ethylene oxide) in the Melt by Small-Angle Neutron Scattering and Molecular Dynamics Simulations. Macromolecules, 2000, 33, 7544-7548.	2.2	49
257	Molecular Dynamics Simulations of Poly(ethylene oxide)/LiI Melts. 2. Dynamic Properties. Macromolecules, 2000, 33, 2273-2283.	2.2	113
258	Conformations and Chain Dimensions of Poly(ethylene oxide) in Aqueous Solution: A Molecular Dynamics Simulation Study. Journal of the American Chemical Society, 2000, 122, 9548-9549.	6.6	100
259	Simulation and QENS Studies of Molecular Dynamics in Aqueous Solutions of 1,2-Dimethoxyethane. Journal of Physical Chemistry B, 2000, 104, 5151-5154.	1.2	17
260	Hydrogenâ€“hydrogen intermolecular structure of polyethylene in the melt. Journal of Chemical Physics, 1999, 110, 8786-8791.	1.2	9
261	Description of thermodynamic properties of liquids over wide ranges of pressure and temperature. Fluid Phase Equilibria, 1998, 146, 63-72.	1.4	0
262	Molecular Dynamics Simulation of 1,2-Dimethoxyethane/Water Solutions. 2. Dynamical Properties. Journal of Physical Chemistry B, 1998, 102, 9565-9570.	1.2	28
263	Quantum Chemistry Based Force Field for Simulations of Poly(propylene oxide) and Its Oligomers. Journal of Physical Chemistry A, 1998, 102, 10318-10323.	1.1	34
264	Molecular Dynamics Simulations of 1,2-Dimethoxyethane/Water Solutions. 1. Conformational and Structural Properties. Journal of Physical Chemistry B, 1998, 102, 5683-5690.	1.2	56
265	Molecular Dynamics Simulations of Poly(ethylene oxide)/LiI Melts. 1. Structural and Conformational Properties. Macromolecules, 1998, 31, 8396-8406.	2.2	146
266	Cation Environment in Molten Lithium Iodide Doped Poly(ethylene oxide). Macromolecules, 1997, 30, 7151-7157.	2.2	64
267	Polymer force fields from ab initio studies of small model molecules: can we achieve chemical accuracy?. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1997, 53, 1273-1283.	2.0	29