Lawrence Pratt

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/8306912/publications.pdf

Version: 2024-02-01

177	13,443	26630	22832
papers	citations	56	112
		h-index	g-index

186	186	186	7321
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Theory of the hydrophobic effect. Journal of Chemical Physics, 1977, 67, 3683-3704.	3.0	797
2	Free Energy of Ionic Hydration. The Journal of Physical Chemistry, 1996, 100, 1206-1215.	2.9	630
3	The pressure dependence of hydrophobic interactions is consistent with the observed pressure denaturation of proteins. Proceedings of the National Academy of Sciences of the United States of America, 1998, 95, 1552-1555.	7.1	562
4	An information theory model of hydrophobic interactions.. Proceedings of the National Academy of Sciences of the United States of America, 1996, 93, 8951-8955.	7.1	520
5	Hydrolysis of Ferric Ion in Water and Conformational Equilibrium. Journal of Physical Chemistry A, 1998, 102, 3565-3573.	2.5	420
6	Hydrophobic Effects and Modeling of Biophysical Aqueous Solution Interfaces. Chemical Reviews, 2002, 102, 2671-2692.	47.7	359
7	Colloquium: Scaled particle theory and the length scales of hydrophobicity. Reviews of Modern Physics, 2006, 78, 159-178.	45.6	349
8	Hydrophobic Effects on a Molecular Scale. Journal of Physical Chemistry B, 1998, 102, 10469-10482.	2.6	331
9	Mechanism of Tetraalkylammonium Headgroup Degradation in Alkaline Fuel Cell Membranes. Journal of Physical Chemistry C, 2008, 112, 3179-3182.	3.1	329
10	MOLECULARTHEORY OFHYDROPHOBICEFFECTS: â€œShe is too mean to have her name repeated.â€• Annual Review of Physical Chemistry, 2002, 53, 409-436.	10.8	305
11	Statistical mechanics of chemical equilibria and intramolecular structures of nonrigid molecules in condensed phases. Journal of Chemical Physics, 1976, 65, 2925-2940.	3.0	286
12	New perspectives on hydrophobic effects. Chemical Physics, 2000, 258, 349-370.	1.9	286
13	Cavities in molecular liquids and the theory of hydrophobic solubilities. Journal of the American Chemical Society, 1990, 112, 5066-5074.	13.7	269
14	A statistical method for identifying transition states in high dimensional problems. Journal of Chemical Physics, 1986, 85, 5045-5048.	3.0	263
15	Origin of Entropy Convergence in Hydrophobic Hydration and Protein Folding. Physical Review Letters, 1996, 77, 4966-4968.	7.8	246
16	The Hydration Number of Li+ in Liquid Water. Journal of the American Chemical Society, 2000, 122, 966-967.	13.7	219
17	Density Functional Theory Study of Degradation of Tetraalkylammonium Hydroxides. Journal of Physical Chemistry C, 2010, 114, 11977-11983.	3.1	216
18	Surface potential of the water liquidâ€“vapor interface. Journal of Chemical Physics, 1988, 88, 3281-3285.	3.0	210

#	Article	IF	Citations
19	Molecular dynamics of the water liquid-vapor interface. The Journal of Physical Chemistry, 1987, 91, 4873-4878.	2.9	208
20	Absolute hydration free energies of ions, ionâ€“water clusters, and quasichemical theory. Journal of Chemical Physics, 2003, 119, 2702-2708.	3.0	200
21	Theory of hydrophobicity: Transient cavities in molecular liquids. Proceedings of the National Academy of Sciences of the United States of America, 1992, 89, 2995-2999.	7.1	192
22	Molecular Theories and Simulation of Ions and Polar Molecules in Water. Journal of Physical Chemistry A, 1998, 102, 7885-7895.	2.5	183
23	Ion sizes and finite-size corrections for ionic-solvation free energies. Journal of Chemical Physics, 1997, 107, 9275-9277.	3.0	181
24	Statistical mechanics of small chain molecules in liquids. I. Effects of liquid packing on conformational structures. Journal of Chemical Physics, 1978, 68, 4202-4212.	3.0	157
25	Hydration Structure and Free Energy of Biomolecularly Specific Aqueous Dications, Including Zn2+ and First Transition Row Metals. Journal of the American Chemical Society, 2004, 126, 1285-1289.	13.7	155
26	From The Cover: Hydration and mobility of HO-(aq). Proceedings of the National Academy of Sciences of the United States of America, 2004, 101, 7229-7233.	7.1	145
27	Effects of soluteâ€“solvent attractive forces on hydrophobic correlations. Journal of Chemical Physics, 1980, 73, 3434-3441.	3.0	138
28	The hydration number of Na+ in liquid water. Fluid Phase Equilibria, 2001, 183-184, 121-132.	2.5	137
29	Free energy of liquid water on the basis of quasichemical theory andab initiomolecular dynamics. Physical Review E, 2003, 68, 041505.	2.1	133
30	Molecular Simulation of Electric Double-Layer Capacitors Based on Carbon Nanotube Forests. Journal of the American Chemical Society, 2009, 131, 12373-12376.	13.7	131
31	Comment on â€˜â€˜Study on the liquidâ€“vapor interface of water. I. Simulation results of thermodynamic properties and orientational structureâ€™â€™. Journal of Chemical Physics, 1989, 90, 5211-5213.	3.0	120
32	Electrostatic Potentials and Free Energies of Solvation of Polar and Charged Molecules. Journal of Physical Chemistry B, 1997, 101, 3017-3020.	2.6	119
33	Ion pair potentials-of-mean-force in water. Biophysical Chemistry, 1994, 51, 147-165.	2.8	117
34	Effective field of a dipole in non-polar polarizable fluids. Molecular Physics, 1980, 40, 347-360.	1.7	109
35	Interaction site cluster series for the Helmholtz free energy and variational principle for chemical equilibria and intramolecular structures. Journal of Chemical Physics, 1977, 66, 147-151.	3.0	104
36	Contact potentials of solution interfaces: phase equilibrium and interfacial electric fields. The Journal of Physical Chemistry, 1992, 96, 25-33.	2.9	103

#	Article	IF	Citations
37	Theory of Hydrophobic Effects. Annual Review of Physical Chemistry, 1985, 36, 433-449.	10.8	101
38	Temperature dependence of the solubility of non-polar gases in water. Biophysical Chemistry, 1999, 78, 21-32.	2.8	98
39	Ab initio molecular dynamics and quasichemical study of H+(aq). Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 6704-6708.	7.1	94
40	Defect structure for proton transport in a triflic acid monohydrate solid. Chemical Physics Letters, 2003, 368, 108-114.	2.6	89
41	Inner shell definition and absolute hydration free energy of K+(aq) on the basis of quasi-chemical theory and ab initio molecular dynamics. Physical Chemistry Chemical Physics, 2004, 6, 1966-1969.	2.8	88
42	Hydration free energy of water. The Journal of Physical Chemistry, 1995, 99, 14188-14194.	2.9	86
43	Comparison of the structure of harmonic aqueous glasses and liquid water. Journal of Chemical Physics, 1987, 87, 6070-6077.	3.0	82
44	Hydrophobic solvation of nonspherical solutes. Journal of Chemical Physics, 1980, 73, 3430-3433.	3.0	81
45	Ion selectivity from local configurations of ligands in solutions and ion channels. Chemical Physics Letters, 2010, 485, 1-7.	2.6	80
46	Marine Oil Fate: Knowledge Gaps, Basic Research, and Development Needs; A Perspective Based on the Deepwater Horizon Spill. Environmental Engineering Science, 2011, 28, 87-93.	1.6	80
47	Design principles for K+ selectivity in membrane transport. Journal of General Physiology, 2011, 137, 479-488.	1.9	74
48	Effects of periodic boundary conditions on equilibrium properties of computer simulated fluids. I. Theory. Journal of Chemical Physics, 1981, 74, 1864-1872.	3.0	73
49	Multistate Gaussian Model for Electrostatic Solvation Free Energies. Journal of the American Chemical Society, 1997, 119, 8523-8527.	13.7	72
50	Hydration theory for molecular biophysics. Advances in Protein Chemistry, 2002, 62, 283-310.	4.4	70
51	Statistical mechanics of small chain molecules in liquids. II. Intermolecular pair correlations for liquidnâ€butane. Journal of Chemical Physics, 1978, 68, 4213-4217.	3.0	65
52	Scaling Atomic Partial Charges of Carbonate Solvents for Lithium Ion Solvation and Diffusion. Journal of Chemical Theory and Computation, 2016, 12, 5709-5718.	5.3	64
53	Is Water the Universal Solvent for Life?. Origins of Life and Evolution of Biospheres, 2012, 42, 405-409.	1.9	61
54	Quasi-Chemical Theory and the Standard Free Energy of H+(aq). Journal of Physical Chemistry A, 2002, 106, 9145-9148.	2.5	60

#	Article	IF	Citations
55	The hydration state of HOâ^'(aq). Chemical Physics Letters, 2003, 380, 530-535.	2.6	59
56	Molecular dynamics test of the Brownian description of Na+ motion in water. Journal of Chemical Physics, 1985, 83, 5832-5836.	3.0	58
57	Quasi-chemical theories of associated liquids. Molecular Physics, 1998, 94, 909-915.	1.7	58
58	Quasi-chemical study of Be2+(aq) speciation. Chemical Physics Letters, 2003, 371, 613-619.	2.6	57
59	Role of attractive methane-water interactions in the potential of mean force between methane molecules in water. Journal of Chemical Physics, 2008, 128, 244512.	3.0	57
60	Deblurred Observation of the Molecular Structure of an Oilâ^'Water Interface. Journal of the American Chemical Society, 2005, 127, 2808-2809.	13.7	56
61	Stability of Cations for Anion Exchange Membrane Fuel Cells. ECS Transactions, 2007, 11, 1173-1180.	0.5	52
62	Effects of periodic boundary conditions on equilibrium properties of computer simulated fluids. II. Application to simple liquids. Journal of Chemical Physics, 1981, 74, 1873-1876.	3.0	51
63	Hydrophobic hydration: Inhomogeneous water structure near nonpolar molecular solutes. Physical Review E, 1996, 53, R4310-R4313.	2.1	50
64	Molecular modeling of trifluoromethanesulfonic acid for solvation theory. Fluid Phase Equilibria, 1998, 150-151, 235-243.	2.5	50
65	Molecular statistical thermodynamics of model micellar aggregates. The Journal of Physical Chemistry, 1984, 88, 2905-2915.	2.9	48
66	Relation between the local field at large distances from a charge or dipole and the dielectric constant. Proceedings of the National Academy of Sciences of the United States of America, 1980, 77, 49-51.	7.1	46
67	Hydration of krypton and consideration of clathrate models of hydrophobic effects from the perspective of quasi-chemical theory. Biophysical Chemistry, 2003, 105, 323-338.	2.8	45
68	Reply to Comment on â€œElectrostatic Potentials and Free Energies of Solvation of Polar and Charged Moleculesâ€• Journal of Physical Chemistry B, 1998, 102, 3841-3843.	2.6	44
69	Variation of the Dissociation Constant of Triflic Acid with Hydration. Journal of Physical Chemistry A, 2001, 105, 6266-6268.	2.5	44
70	Role of fluctuations in a snug-fit mechanism of KcsA channel selectivity. Journal of Chemical Physics, 2006, 125, 024701.	3.0	44
71	Theoretical Calculation of the Water Ion Product KW. Journal of the American Chemical Society, 1995, 117, 1625-1628.	13.7	43
72	Solvation Free Energy Calculations Using a Continuum Dielectric Model for the Solvent and Gradient-Corrected Density Functional Theory for the Solute. The Journal of Physical Chemistry, 1996, 100, 1515-1523.	2.9	43

#	Article	IF	Citations
73	Quasi-Chemical Theory for the Statistical Thermodynamics of the Hard-Sphere Fluidâ€. Journal of Physical Chemistry B, 2001, 105, 11662-11668.	2.6	43
74	Molecular Realism in Default Models for Information Theories of Hydrophobic Effects. Journal of Physical Chemistry B, 1999, 103, 3520-3523.	2.6	42
75	Balancing local order and long-ranged interactions in the molecular theory of liquid water. Journal of Chemical Physics, 2007, 127, 144508.	3.0	42
76	Contrasting Nonaqueous against Aqueous Solvation on the Basis of Scaled-Particle Theory. Journal of Physical Chemistry B, 2007, 111, 9330-9336.	2.6	42
77	Structural Models and Molecular Thermodynamics of Hydration ofÂIons and Small Molecules. Annual Reports in Computational Chemistry, 2012, 8, 71-127.	1.7	42
78	Dielectric Relaxation of Ethylene Carbonate and Propylene Carbonate from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2016, 120, 1849-1853.	2.6	42
79	Hydrophobic interactions and osmotic second virial coefficients for methanol in water. Journal of Solution Chemistry, 1980, 9, 1-17.	1.2	41
80	Monte carlo study of a simple model for micelle structure. Chemical Physics Letters, 1981, 79, 436-440.	2.6	39
81	Molecular-scale hydrophobic interactions between hard-sphere reference solutes are attractive and endothermic. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 20557-20562.	7.1	38
82	An analysis of molecular packing and chemical association in liquid water using quasichemical theory. Journal of Chemical Physics, 2006, 124, 224502.	3.0	37
83	Boundary integral methods for the Poisson equation of continuum dielectric solvation models. International Journal of Quantum Chemistry, 1997, 64, 121-141.	2.0	36
84	Discretized propagators, Hartree, and Hartreeâ€“Fock equations, and the Hohenbergâ€“Kohn theorem. Journal of Chemical Physics, 1985, 82, 856-859.	3.0	35
85	Non-van der Waals Treatment of the Hydrophobic Solubilities of CF4. Journal of the American Chemical Society, 2007, 129, 10133-10140.	13.7	35
86	A method for systematic inclusion of electron correlation in density functionals. Journal of Chemical Physics, 1985, 83, 4024-4028.	3.0	34
87	Quasi-chemical theory and implicit solvent models for simulations. , 1999, , .		34
88	Solution Influence on Biomolecular Equilibria: Nucleic Acid Base Associations. Journal of Biomolecular Structure and Dynamics, 1984, 1, 1257-1280.	3.5	33
89	Interaction of a sodium ion with the water liquid-vapor interface. Chemical Physics, 1989, 129, 209-212.	1.9	33
90	Molecular Dynamics of Lithium Ion Transport in a Model Solid Electrolyte Interphase. Scientific Reports, 2018, 8, 10736.	3.3	33

#	Article	IF	Citations
91	Case study of Rb+(aq), quasi-chemical theory of ion hydration, and the no split occupancies rule. Annual Reports on the Progress of Chemistry Section C, 2013, 109, 266.	4.4	31
92	Effective intramolecular potentials for molecular bromine in argon. Comparison of theory with simulation. Journal of Chemical Physics, 1980, 72, 4045-4048.	3.0	30
93	Dielectric saturation of liquid propylene carbonate in electrical energy storage applications. Journal of Chemical Physics, 2010, 132, 044701.	3.0	30
94	Beryllium Displacement of H+ from Strong Hydrogen Bonds. Angewandte Chemie - International Edition, 2007, 46, 2669-2671.	13.8	29
95	Potential Distribution Methods and Free Energy Models of Molecular Solutions. Springer Series in Chemical Physics, 2007, , 323-351.	0.2	28
96	Quasichemical theory with a soft cutoff. Journal of Chemical Physics, 2009, 130, 054113.	3.0	28
97	Hydration Mimicry by Membrane Ion Channels. Annual Review of Physical Chemistry, 2020, 71, 461-484.	10.8	27
98	Monte Carlo calculation of the molecular structure of surfactant bilayers. The Journal of Physical Chemistry, 1984, 88, 6048-6052.	2.9	25
99	Introduction:Â Water. Chemical Reviews, 2002, 102, 2625-2626.	47.7	25
100	Molecular Theory and the Effects of Solute Attractive Forces on Hydrophobic Interactions. Journal of Physical Chemistry B, 2016, 120, 1864-1870.	2.6	25
101	Thermodynamics of ion binding and occupancy in potassium channels. Chemical Science, 2021, 12, 8920-8930.	7.4	25
102	Statistical theory of electron densities. Journal of Chemical Physics, 1988, 88, 1818-1823.	3.0	23
103	Statistical Analyses of Hydrophobic Interactions: A Mini-Review. Journal of Physical Chemistry B, 2016, 120, 6455-6460.	2.6	22
104	Anomalous Potential-Dependent Friction on Au(111) Measured by AFM. Langmuir, 2018, 34, 801-806.	3.5	22
105	[3] Theoretical and computational studies of hydrophobic interactions. Methods in Enzymology, 1986, 127, 48-63.	1.0	21
106	Self-consistent molecular field theory for packing in classical liquids. Physical Review E, 2003, 68, 021505.	2.1	21
107	Triboelectricity Generation from Vertically Aligned Carbon Nanotube Arrays. ACS Applied Materials & Interfaces, 2016, 8, 27454-27457.	8.0	21
108	Hard-sphere solids with one fluid component. The Journal of Physical Chemistry, 1981, 85, 3221-3224.	2.9	20

#	Article	IF	Citations
109	Salt effects on the surface tensions of dilute electrolyte solutions: The influence of nonzero relative solubility of the salt between the coexisting phases. Journal of Chemical Physics, 1984, 80, 6225-6233.	3.0	20
110	Hydration of Kr(aq) in Dilute and Concentrated Solutions. Journal of Physical Chemistry B, 2015, 119, 9098-9102.	2.6	20
111	Molecular theory of surfactant micelles in aqueous solution. Advances in Colloid and Interface Science, 1986, 26, 69-97.	14.7	18
112	Molecular dynamics of a dilute solution of hydrogen in palladium. Physical Review B, 1989, 39, 13170-13174.	3.2	18
113	Spectroscopic studies of surface and subsurface hydrogen/metal systems. Journal of Chemical Physics, 1992, 97, 5177-5181.	3.0	16
114	Distribution of Binding Energies of a Water Molecule in the Water Liquidâ^'Vapor Interface. Journal of Physical Chemistry B, 2009, 113, 4147-4151.	2.6	16
115	Utility of chemical computations in predicting solution free energies of metal ions. Molecular Simulation, 2018, 44, 110-116.	2.0	16
116	Comment on the structure of a simple liquid solvent near a nâ€butane solute molecule. Journal of Chemical Physics, 1980, 73, 1002-1003.	3.0	15
117	Interfaces of propylene carbonate. Journal of Chemical Physics, 2013, 138, 114708.	3.0	15
118	Assessment of Simple Models for Molecular Simulation of Ethylene Carbonate and Propylene Carbonate as Solvents for Electrolyte Solutions. Topics in Current Chemistry, 2018, 376, 7.	5.8	15
119	Quasi-chemical theory for anion hydration and specific ion effects: <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si36.svg"><mml:mrow><mml:msup><mml:mrow><mml:mi mathvariant="normal">Cl</mml:mi></mml:mrow><mml:mrow><mml:mo>-</mml:mo></mml:mrow></mml:msup></mml:mrow></mml:math> vs. <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si37.svg"><mml:mrow><mml:msup><mml:mrow><mml:mi mathvariant="normal">F</mml:mi></mml:mrow></mml:msup></mml:mrow></mml:math>	2.1	15
120	Theory for surface structure of dilute electrolyte solutions. Journal of Chemical Physics, 1982, 76, 3782-3791.	3.0	14
121	Free energy of nucleating droplets via cluster-integral series. Physical Review A, 1983, 28, 2482-2490.	2.5	13
122	Generalizations of the Fuoss approximation for ion pairing. Journal of Chemical Physics, 2011, 134, 054502.	3.0	13
123	Vertically-Aligned Carbon Nanotube Arrays as Binder-Free Supports for Nickel Cobaltite based Faradaic Supercapacitor Electrodes. Electrochimica Acta, 2017, 236, 408-416.	5.2	13
124	Pairing of 1-hexyl-3-methylimidazolium and tetrafluoroborate ions in n-pentanol. Journal of Chemical Physics, 2012, 137, 174501.	3.0	12
125	Quasi-chemical theory of Fâ^'(aq): The â€œno split occupancies ruleâ€•revisited. Journal of Chemical Physics, 2017, 147, 161728.	3.0	12
126	Quasi-Chemical Theory with Cluster Sampling from Ab Initio Molecular Dynamics: Fluoride (F^{â€“}) Anion Hydration. Journal of Physical Chemistry A, 2018, 122, 9806-9812.	2.5	12

#	Article	IF	Citations
127	Role of Solute Attractive Forces in the Atomic-Scale Theory of Hydrophobic Effects. Journal of Physical Chemistry B, 2018, 122, 6272-6276.	2.6	12
128	Slow decay of ion correlations parallel to an electrolyte solution surface. Journal of Chemical Physics, 1982, 77, 1070-1072.	3.0	11
129	A new Monte Carlo method for direct estimation of cluster partition functions. Application to micellar aggregates. Journal of Chemical Physics, 1982, 77, 979-985.	3.0	11
130	Effect of PEG End-Group Hydrophobicity on Lysozyme Interactions in Solution Characterized by Light Scattering. Langmuir, 2011, 27, 13713-13718.	3.5	11
131	Concentration dependence of the Flory-Huggins interaction parameter in aqueous solutions of capped PEO chains. Journal of Chemical Physics, 2014, 141, 244908.	3.0	11
132	Hydrophilic Interactions Dominate the Inverse Temperature Dependence of Polypeptide Hydration Free Energies Attributed to Hydrophobicity. Journal of Physical Chemistry Letters, 2020, 11, 9965-9970.	4.6	11
133	Multiple nucleation pathways near triple points of Arâ€“Kr mixtures. Journal of Chemical Physics, 1984, 80, 1605-1609.	3.0	10
134	Discretized propagators in Hartree and Hartreeâ€“Fock theory. II. Responses to static electric and magnetic fields. Journal of Chemical Physics, 1985, 82, 5084-5088.	3.0	10
135	Monte Carlo integration of density functional theory: Fermions in a harmonic well. Chemical Physics Letters, 1988, 148, 313-316.	2.6	10
136	Ground state densities from electron propagators: Optimized Thomasâ€“Fermi approximation for short wavelength modes. Journal of Chemical Physics, 1990, 92, 6687-6696.	3.0	10
137	Construction of simulation wave functions for aqueous species: D3O+. Journal of Chemical Physics, 1998, 109, 8783-8789.	3.0	10
138	Water adsorption and dissociation on BeO(001) and (100) surfaces. Surface Science, 2007, 601, 1608-1614.	1.9	10
139	Dissolution Kinetics of [Hmim][BF₄] Ionic Liquid Droplets in 1-Pentanol. Journal of Physical Chemistry C, 2009, 113, 16458-16463.	3.1	10
140	[4] Theoretical methods for obtaining free energies of biomolecular equilibria in aqueous solutions. Methods in Enzymology, 1986, 127, 64-78.	1.0	9
141	Estimate of the probability of diffusional misordering in high-speed DNA sequencing. The Journal of Physical Chemistry, 1993, 97, 10254-10255.	2.9	9
142	Reaction field spectral shifts with semiempirical molecular orbital theory. International Journal of Quantum Chemistry, 1997, 64, 143-155.	2.0	9
143	Treatment of electrostatic interactions in computer simulations and calculation of thermodynamic properties such as free energies and pressures. , 1999, , .		9
144	Cages of Water Coordinating Kr in Aqueous Solution. Journal of Physical Chemistry A, 2003, 107, 11267-11270.	2.5	9

#	Article	IF	Citations
145	AIMD Results for a Concentrated Solution of Tetra-ethylammonium Tetra-fluoroborate in Propylene Carbonate. ECS Transactions, 2015, 66, 1-5.	0.5	9
146	Thermodynamics of Hydration from the Perspective of the Molecular Quasichemical Theory of Solutions. Journal of Physical Chemistry B, 2021, 125, 8294-8304.	2.6	9
147	Hydrated Anions: From Clusters to Bulk Solution with Quasi-Chemical Theory. Accounts of Chemical Research, 2022, 55, 2201-2212.	15.6	9
148	Fluctuation method for calculation of elastic constants of solids. Journal of Chemical Physics, 1987, 87, 1245-1247.	3.0	8
149	Communication: Direct observation of a hydrophobic bond in loop closure of a capped (â€“OCH2CH2â€“)n oligomer in water. Journal of Chemical Physics, 2010, 133, 231102.	3.0	8
150	Molecular Dynamics Simulations of Lithium Ion Transport through a Model Solid Electrolyte Interphase (SEI) Layer. ECS Transactions, 2017, 77, 1155-1162.	0.5	8
151	Theories of Hydrophobic Effects and the Description of Free Volume in Complex Liquids. , 1999, , 407-420.		8
152	Disentanglement of hydrophobic and electrostatic contributions to the film pressures of ionic surfactants. Faraday Symposia of the Chemical Society, 1982, 17, 129.	0.5	7
153	Comparison of electron density functional models. Molecular Physics, 1994, 82, 245-261.	1.7	7
154	Molecular Simulation Results on Charged Carbon Nanotube Forestâ€Based Supercapacitors. ChemSusChem, 2018, 11, 1927-1932.	6.8	7
155	Statistical determination of normal modes. Journal of Chemical Education, 1987, 64, 425.	2.3	6
156	Distributions of extreme contributions to binding energies of molecules in liquids. Chemical Physics Letters, 2010, 487, 24-27.	2.6	6
157	Design principles for K+ selectivity in membrane transport. Journal of General Physiology, 2011, 138, 279-279.	1.9	5
158	Comparison of single-ion molecular dynamics in common solvents. Journal of Chemical Physics, 2018, 148, 222821.	3.0	5
159	Molecular-Scale Description of SPAN80 Desorption from a Squalaneâ€“Water Interface. Journal of Physical Chemistry B, 2018, 122, 3378-3383.	2.6	5
160	Free Energies of Hydrated Halide Anions: High Through-Put Computations on Clusters to Treat Rough Energy-Landscapes. Molecules, 2021, 26, 3087.	3.8	5
161	Remarks on â€œthe field far from a charge and a dipoleâ€. Chemical Physics Letters, 1981, 78, 201.	2.6	4
162	Connection between central force model treatment of polyatomic molecular liquids and the interaction site cluster expansion. Molecular Physics, 1981, 43, 1163-1173.	1.7	4

#	Article	IF	Citations
163	Hydrophobic interaction of amphiphilic ions with waterâ€“hydrocarbon liquid interfaces. Journal of Chemical Physics, 1984, 81, 579-580.	3.0	4
164	Lower bound on the ground-state energies of atoms and molecules by variational quantum Monte Carlo methods. Physical Review A, 1989, 40, 6077-6079.	2.5	4
165	A simple effective Hamiltonian for low-frequency linear responses. Chemical Physics Letters, 1993, 203, 399-403.	2.6	4
166	Multiscale Theory in the Molecular Simulation of Electrolyte Solutions. Journal of Physical Chemistry B, 2014, 118, 7730-7738.	2.6	4
167	Theory of electrolyte solution interfaces at finite dilution. Journal of Chemical Physics, 1983, 78, 5129-5137.	3.0	3
168	Tests of Dielectric Model Descriptions of Chemical Charge Displacements in Water. ACS Symposium Series, 1994, , 60-70.	0.5	3
169	Concentrating Low-Level Tritiated Water through Isotope Exchange. Fusion Science and Technology, 2000, 37, 124-130.	0.6	3
170	Loop-Closure and Gaussian Models of Collective Structural Characteristics of Capped PEO Oligomers in Water. Journal of Physical Chemistry B, 2015, 119, 8863-8867.	2.6	3
171	Statistical theory of electron densities: multiple scattering perturbation theory. Proceedings of the Royal Society A, 1991, 435, 245-255.	0.9	2
172	Statistical theory of electron densities at nonzero temperatures. Canadian Journal of Chemistry, 1992, 70, 478-481.	1.1	2
173	Reduction of diffusion broadening in flow by analysis of time-gated single-molecule data. Analyst, The, 2010, 135, 1333.	3.5	1
174	Introduction to Special Issue on Water and Associated Liquids. Journal of Statistical Physics, 2011, 145, 207-208.	1.2	1
175	Boundary integral methods for the Poisson equation of continuum dielectric solvation models. International Journal of Quantum Chemistry, 1997, 64, 121-141.	2.0	1
176	Hydrophobic Effect. , 2015, , 1152-1155.		0
177	Shapes of Nonsymmetric Capillary Bridges. Journal of Physical Chemistry B, 2021, 125, 12378-12383.	2.6	0