Lawrence Pratt

List of Publications by Year in descending order

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177 13,443 papers citations

56 h-index 22832 112 g-index

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

#	Article	IF	CITATIONS
1	Hydrated Anions: From Clusters to Bulk Solution with Quasi-Chemical Theory. Accounts of Chemical Research, 2022, 55, 2201-2212.	15.6	9
2	Thermodynamics of ion binding and occupancy in potassium channels. Chemical Science, 2021, 12, 8920-8930.	7.4	25
3	Free Energies of Hydrated Halide Anions: High Through-Put Computations on Clusters to Treat Rough Energy-Landscapes. Molecules, 2021, 26, 3087.	3.8	5
4	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
5	Shapes of Nonsymmetric Capillary Bridges. Journal of Physical Chemistry B, 2021, 125, 12378-12383.	2.6	0
6	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
7	Hydration Mimicry by Membrane Ion Channels. Annual Review of Physical Chemistry, 2020, 71, 461-484. Quasi-chemical theory for anion hydration and specific ion effects: <mml:math< td=""><td>10.8</td><td>27</td></mml:math<>	10.8	27
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11	Molecular-Scale Description of SPAN80 Desorption from a Squalane–Water Interface. Journal of Physical Chemistry B, 2018, 122, 3378-3383.	2.6	5
12	Molecular Simulation Results on Charged Carbon Nanotube Forestâ€Based Supercapacitors. ChemSusChem, 2018, 11, 1927-1932.	6.8	7
13	Anomalous Potential-Dependent Friction on Au(111) Measured by AFM. Langmuir, 2018, 34, 801-806.	3.5	22
14	Utility of chemical computations in predicting solution free energies of metal ions. Molecular Simulation, 2018, 44, 110-116.	2.0	16
15	Quasi-Chemical Theory with Cluster Sampling from Ab Initio Molecular Dynamics: Fluoride (F [–]) Anion Hydration. Journal of Physical Chemistry A, 2018, 122, 9806-9812.	2.5	12
16	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
17	Molecular Dynamics of Lithium Ion Transport in a Model Solid Electrolyte Interphase. Scientific Reports, 2018, 8, 10736.	3.3	33
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23	Statistical Analyses of Hydrophobic Interactions: A Mini-Review. Journal of Physical Chemistry B, 2016, 120, 6455-6460.	2.6	22
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37	Structural Models and Molecular Thermodynamics of Hydration ofÂlons and Small Molecules. Annual Reports in Computational Chemistry, 2012, 8, 71-127.	1.7	42
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39	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
40	Introduction to Special Issue on Water and Associated Liquids. Journal of Statistical Physics, 2011, 145, 207-208.	1.2	1
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47	Density Functional Theory Study of Degradation of Tetraalkylammonium Hydroxides. Journal of Physical Chemistry C, 2010, 114, 11977-11983.	3.1	216
48	Dielectric saturation of liquid propylene carbonate in electrical energy storage applications. Journal of Chemical Physics, 2010, 132, 044701.	3.0	30
49	Reduction of diffusion broadening in flow by analysis of time-gated single-molecule data. Analyst, The, 2010, 135, 1333.	3.5	1
50	Quasichemical theory with a soft cutoff. Journal of Chemical Physics, 2009, 130, 054113.	3.0	28
51	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
52	Dissolution Kinetics of [Hmim][BF ₄] Ionic Liquid Droplets in 1-Pentanol. Journal of Physical Chemistry C, 2009, 113, 16458-16463.	3.1	10
53	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
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55	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
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61	Beryllium Displacement of H+ from Strong Hydrogen Bonds. Angewandte Chemie - International Edition, 2007, 46, 2669-2671.	13.8	29
62	Water adsorption and dissociation on BeO(001) and (100) surfaces. Surface Science, 2007, 601, 1608-1614.	1.9	10
63	Colloquium: Scaled particle theory and the length scales of hydrophobicity. Reviews of Modern Physics, 2006, 78, 159-178.	45.6	349
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66	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
67	Deblurred Observation of the Molecular Structure of an Oilâ°'Water Interface. Journal of the American Chemical Society, 2005, 127, 2808-2809.	13.7	56
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74	Quasi-chemical study of Be2+(aq) speciation. Chemical Physics Letters, 2003, 371, 613-619.	2.6	57
75	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
76	Free energy of liquid water on the basis of quasichemical theory andab initiomolecular dynamics. Physical Review E, 2003, 68, 041505.	2.1	133
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78	Self-consistent molecular field theory for packing in classical liquids. Physical Review E, 2003, 68, 021505.	2.1	21
79	Hydration theory for molecular biophysics. Advances in Protein Chemistry, 2002, 62, 283-310.	4.4	70
80	Quasi-Chemical Theory and the Standard Free Energy of H+(aq). Journal of Physical Chemistry A, 2002, 106, 9145-9148.	2.5	60
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84	Variation of the Dissociation Constant of Triflic Acid with Hydration. Journal of Physical Chemistry A, 2001, 105, 6266-6268.	2.5	44
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92	Quasi-chemical theory and implicit solvent models for simulations. , 1999, , .		34
93	Treatment of electrostatic interactions in computer simulations and calculation of thermodynamic properties such as free energies and pressures. , 1999, , .		9
94	Theories of Hydrophobic Effects and the Description of Free Volume in Complex Liquids. , 1999 , , $407-420$.		8
95	Molecular modeling of trifluoromethanesulfonic acid for solvation theory. Fluid Phase Equilibria, 1998, 150-151, 235-243.	2.5	50
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100	Hydrolysis of Ferric Ion in Water and Conformational Equilibrium. Journal of Physical Chemistry A, 1998, 102, 3565-3573.	2.5	420
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