Thomas L Beck

List of Publications by Year
in descending order

56 papers	1,886 citations	257450 24 h-index	276875 41 g-index
61 all docs	61 docs citations	61 times ranked	1418 citing authors

#	Article	IF	Citations
1	Deep neural network based quantum simulations and quasichemical theory for accurate modeling of molten salt thermodynamics. Chemical Science, 2022, 13, 8265-8273.	7.4	3
2	Quantum Simulations of Hydrogen Bonding Effects in Glycerol Carbonate Electrolyte Solutions. Journal of Physical Chemistry B, 2021, 125, 2157-2166.	2.6	7
3	Biphasic, Membrane-Free Zn/Phenothiazine Battery: Effects of Hydrophobicity of Redox Materials on Cyclability. , 2021, 3, 337-343.		16
4	Tribute to Lawrence R. Pratt. Journal of Physical Chemistry B, 2021, 125, 4925-4927.	2.6	0
5	Condensed Phase Water Molecular Multipole Moments from Deep Neural Network Models Trained on Ab Initio Simulation Data. Journal of Physical Chemistry Letters, 2021, 12, 10310-10317.	4.6	11
6	Specific Ion Solvation and Pairing Effects in Glycerol Carbonate. Journal of Physical Chemistry B, 2021, 125, 13635-13643.	2.6	4
7	Absolute ion hydration free energy scale and the surface potential of water via quantum simulation. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 30151-30158.	7.1	14
8	Investigating partitioning of freeversusmacrocycle bound guest into a model POPC lipid bilayer. RSC Advances, 2020, 10, 15148-15153.	3.6	2
9	Molecular Basis of CLC Antiporter Inhibition by Fluoride. Journal of the American Chemical Society, 2020, 142, 7254-7258.	13.7	20
10	The Importance of the Water Molecular Quadrupole for Estimating Interfacial Potential Shifts Acting on Ions Near the Liquidâ€“Vapor Interface. Journal of Physical Chemistry B, 2019, 123, 3348-3358.	2.6	34
11	Re-examining the tetraphenyl-arsonium/tetraphenyl-borate (TATB) hypothesis for single-ion solvation free energies. Journal of Chemical Physics, 2018, 148, 222830.	3.0	22
12	Deconstructing Free Energies in the Law of Matching Water Affinities. Journal of Physical Chemistry B, 2017, 121, 2189-2201.	2.6	17
13	Novel Liposome-Based Surface-Enhanced Raman Spectroscopy (SERS) Substrate. Journal of Physical Chemistry Letters, 2017, 8, 2639-2646.	4.6	30
14	Structure and polarization near the Li+ ion in ethylene and propylene carbonates. Journal of Chemical Physics, 2017, 147, 161710.	3.0	20
15	Toward a quantitative theory of Hofmeister phenomena: From quantum effects to thermodynamics. Current Opinion in Colloid and Interface Science, 2016, 23, 110-118.	7.4	55
16	Free Energies of Ion Binding in the Bacterial CLC-ec1 Chloride Transporter with Implications for the Transport Mechanism and Selectivity. Journal of Physical Chemistry B, 2016, 120, 3129-3139.	2.6	12
17	Models of Ion Solvation Thermodynamics in Ethylene Carbonate and Propylene Carbonate. Journal of Physical Chemistry B, 2016, 120, 1497-1508.	2.6	28
18	A real-space stochastic density matrix approach for density functional electronic structure. Physical Chemistry Chemical Physics, 2015, 17, 31472-31479.	2.8	1

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19	The thermodynamics of proton hydration and the electrochemical surface potential of water. Journal of Chemical Physics, 2014, 141, 18C512.	3.0	36
20	Quasichemical analysis of the cluster-pair approximation for the thermodynamics of proton hydration. Journal of Chemical Physics, 2014, 140, 224507.	3.0	25
21	Length scales and interfacial potentials in ion hydration. Journal of Chemical Physics, 2013, 139, 044504.	3.0	34
22	Temperature Dependence of Gramicidin Channel Transport and Structure. Journal of Physical Chemistry C, 2013, 117, 3701-3712.	3.1	8
23	The influence of water interfacial potentials on ion hydration in bulk water and near interfaces. Chemical Physics Letters, 2013, 561-562, 1-13.	2.6	102
24	Free energy partitioning analysis of the driving forces that determine ion density profiles near the water liquid-vapor interface. Journal of Chemical Physics, 2012, 136, 104503.	3.0	44
25	Solving the SchrÃ¶dinger Equation on Real-Space Grids and with Random Walks. , 2011, , 271-311.		0
26	A Local Entropic Signature of Specific Ion Hydration. Journal of Physical Chemistry B, 2011, 115, 9776-9781.	2.6	45
27	Hydration Free Energies by Energetic Partitioning of the Potential Distribution Theorem. Journal of Statistical Physics, 2011, 145, 335-354.	1.2	28
28	An Information Theory Approach to Nonlinear, Nonequilibrium Thermodynamics. Journal of Statistical Physics, 2011, 145, 385-409.	1.2	11
29	Polarization and charge transfer in the hydration of chloride ions. Journal of Chemical Physics, 2010, 132, 014502.	3.0	84
30	Quasichemical and structural analysis of polarizable anion hydration. Journal of Chemical Physics, 2010, 132, 014505.	3.0	62
31	Transpath: A computational method for locating ion transit pathways through membrane proteins. Proteins: Structure, Function and Bioinformatics, 2008, 71, 1349-1359.	2.6	10
32	Modeling molecular and ionic absolute solvation free energies with quasichemical theory bounds. Journal of Chemical Physics, 2008, 129, 134505.	3.0	28
33	Efficient multiscale algorithms for solution of self-consistent eigenvalue problems in real space. Physical Review B, 2007, 75, .	3.2	11
34	Equilibrium and Dynamical Fourier Path Integral Methods. Advances in Chemical Physics, 2007, , 61-127.	0.3	165
35	Proton pathways and H+/Clâ^' stoichiometry in bacterial chloride transporters. Proteins: Structure, Function and Bioinformatics, 2007, 68, 26-33.	2.6	47
36	Quantum Contributions to Free Energy Changes in Fluids. Springer Series in Chemical Physics, 2007, , 389-422.	0.2	2

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37	Nonlinear multigrid eigenvalue solver utilizing nonorthogonal localized orbitals. Physica Status Solidi (B): Basic Research, 2006, 243, 1054-1062.	1.5	8
38	Comment on ion transit pathways and gating in ClC chloride channels. Proteins: Structure, Function and Bioinformatics, 2005, 62, 553-554.	2.6	4
39	Ion transit pathways and gating in ClC chloride channels. Proteins: Structure, Function and Bioinformatics, 2004, 57, 414-421.	2.6	52
40	MULTISCALE ALGORITHMS FOR EIGENVALUE PROBLEMS. Journal of Theoretical and Computational Chemistry, 2003, 02, 553-561.	1.8	6
41	Real-space mesh techniques in density-functional theory. Reviews of Modern Physics, 2000, 72, 1041-1080.	45.6	432
42	Efficient real-space solution of the Kohnâ€“Sham equations with multiscale techniques. Journal of Chemical Physics, 2000, 112, 9223-9228.	3.0	36
43	Computer Simulations of Interphases and Solute Transfer in Liquid and Size Exclusion Chromatography. ACS Symposium Series, 1999, , 67-81.	0.5	4
44	Multigrid high-order mesh refinement techniques for composite grid electrostatics calculations. Journal of Computational Chemistry, 1999, 20, 1731-1739.	3.3	15
45	Multiscale techniques for electrostatics and eigenvalue problems in real space. , 1999, , .		0
46	Vaporâ^'Liquid Equilibria of Binary and Ternary Mixtures Containing Methane, Ethane, and Carbon Dioxide from Gibbs Ensemble Simulations. Journal of Physical Chemistry B, 1998, 102, 7627-7631.	2.6	28
47	Multigrid methods in density functional theory. International Journal of Quantum Chemistry, 1997, 61, 341-348.	2.0	19
48	Real-space multigrid solution of electrostatics problems and the Kohn-Sham equations. International Journal of Quantum Chemistry, 1997, 65, 477-486.	2.0	26
49	Microscopic Simulation of Solute Transfer in Reversed Phase Liquid Chromatography. The Journal of Physical Chemistry, 1996, 100, 5931-5934.	2.9	83
50	Prediction of liquidâ€“liquid phase equilibria of He+H2 mixtures by NpT molecular dynamics simulations. Journal of Chemical Physics, 1996, 105, 2424-2428.	3.0	8
51	Methods of Single-Step and Multistep Particle Switching in Simulations of Mixtures. The Journal of Physical Chemistry, 1996, 100, 16002-16005.	2.9	1
52	Application of a distributed nucleus approximation in grid based minimization of the Kohnâ€“Sham energy functional. Journal of Chemical Physics, 1995, 103, 227-233.	3.0	32
53	Determination of excess Gibbs free energy of quantum mixtures by path integral Monte Carlo simulations. Molecular Physics, 1995, 86, 225-233.	1.7	11
54	Monte Carlo evaluation of real time coherent state path integrals. Journal of Chemical Physics, 1992, 96, 2966-2977.	3.0	23

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55	Quantum path integral extension of Widomâ€™s test particle method for chemical potentials with application to isotope effects on hydrogen solubilities in model solids. Journal of Chemical Physics, 1992, 96, 7175-7177.	3.0	14
56	Dynamics of diffusion in small cluster systems. Journal of Chemical Physics, 1990, 93, 1347-1357.	3.0	41