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	Real-space mesh techniques in density-functional theory. Reviews of Modern Physics, 2000, 72, 1041-1080.	45.6	432
2	Equilibrium and Dynamical Fourier Path Integral Methods. Advances in Chemical Physics, 2007, , 61-127.	0.3	165
3	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
4	Polarization and charge transfer in the hydration of chloride ions. Journal of Chemical Physics, 2010, 132, 014502.	3.0	84
5	Microscopic Simulation of Solute Transfer in Reversed Phase Liquid Chromatography. The Journal of Physical Chemistry, 1996, 100, 5931-5934.	2.9	83
6	Quasichemical and structural analysis of polarizable anion hydration. Journal of Chemical Physics, 2010, 132, 014505.	3.0	62
7	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
8	Ion transit pathways and gating in ClC chloride channels. Proteins: Structure, Function and Bioinformatics, 2004, 57, 414-421.	2.6	52
9	Proton pathways and H+/Clâ^' stoichiometry in bacterial chloride transporters. Proteins: Structure, Function and Bioinformatics, 2007, 68, 26-33.	2.6	47
10	A Local Entropic Signature of Specific Ion Hydration. Journal of Physical Chemistry B, 2011, 115, 9776-9781.	2.6	45
11	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
12	Dynamics of diffusion in small cluster systems. Journal of Chemical Physics, 1990, 93, 1347-1357.	3.0	41
13	Efficient real-space solution of the Kohnâ€“Sham equations with multiscale techniques. Journal of Chemical Physics, 2000, 112, 9223-9228.	3.0	36
14	The thermodynamics of proton hydration and the electrochemical surface potential of water. Journal of Chemical Physics, 2014, 141, 18C512.	3.0	36
15	Length scales and interfacial potentials in ion hydration. Journal of Chemical Physics, 2013, 139, 044504.	3.0	34
16	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
17	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
18	Novel Liposome-Based Surface-Enhanced Raman Spectroscopy (SERS) Substrate. Journal of Physical Chemistry Letters, 2017, 8, 2639-2646.	4.6	30

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19	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
20	Modeling molecular and ionic absolute solvation free energies with quasichemical theory bounds. Journal of Chemical Physics, 2008, 129, 134505.	3.0	28
21	Hydration Free Energies by Energetic Partitioning of the Potential Distribution Theorem. Journal of Statistical Physics, 2011, 145, 335-354.	1.2	28
22	Models of Ion Solvation Thermodynamics in Ethylene Carbonate and Propylene Carbonate. Journal of Physical Chemistry B, 2016, 120, 1497-1508.	2.6	28
23	Real-space multigrid solution of electrostatics problems and the Kohn-Sham equations. International Journal of Quantum Chemistry, 1997, 65, 477-486.	2.0	26
24	Quasichemical analysis of the cluster-pair approximation for the thermodynamics of proton hydration. Journal of Chemical Physics, 2014, 140, 224507.	3.0	25
25	Monte Carlo evaluation of real time coherent state path integrals. Journal of Chemical Physics, 1992, 96, 2966-2977.	3.0	23
26	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
27	Structure and polarization near the Li+ ion in ethylene and propylene carbonates. Journal of Chemical Physics, 2017, 147, 161710.	3.0	20
28	Molecular Basis of CLC Antiporter Inhibition by Fluoride. Journal of the American Chemical Society, 2020, 142, 7254-7258.	13.7	20
29	Multigrid methods in density functional theory. International Journal of Quantum Chemistry, 1997, 61, 341-348.	2.0	19
30	Deconstructing Free Energies in the Law of Matching Water Affinities. Journal of Physical Chemistry B, 2017, 121, 2189-2201.	2.6	17
31	Biphasic, Membrane-Free Zn/Phenothiazine Battery: Effects of Hydrophobicity of Redox Materials on Cyclability. , 2021, 3, 337-343.		16
32	Multigrid high-order mesh refinement techniques for composite grid electrostatics calculations. Journal of Computational Chemistry, 1999, 20, 1731-1739.	3.3	15
33	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
34	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
35	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
36	Determination of excess Gibbs free energy of quantum mixtures by path integral Monte Carlo simulations. Molecular Physics, 1995, 86, 225-233.	1.7	11

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37	Efficient multiscale algorithms for solution of self-consistent eigenvalue problems in real space. Physical Review B, 2007, 75, .	3.2	11
38	An Information Theory Approach to Nonlinear, Nonequilibrium Thermodynamics. Journal of Statistical Physics, 2011, 145, 385-409.	1.2	11
39	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
40	Transpath: A computational method for locating ion transit pathways through membrane proteins. Proteins: Structure, Function and Bioinformatics, 2008, 71, 1349-1359.	2.6	10
41	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
42	Nonlinear multigrid eigenvalue solver utilizing nonorthogonal localized orbitals. Physica Status Solidi (B): Basic Research, 2006, 243, 1054-1062.	1.5	8
43	Temperature Dependence of Gramicidin Channel Transport and Structure. Journal of Physical Chemistry C, 2013, 117, 3701-3712.	3.1	8
44	Quantum Simulations of Hydrogen Bonding Effects in Glycerol Carbonate Electrolyte Solutions. Journal of Physical Chemistry B, 2021, 125, 2157-2166.	2.6	7
45	MULTISCALE ALGORITHMS FOR EIGENVALUE PROBLEMS. Journal of Theoretical and Computational Chemistry, 2003, 02, 553-561.	1.8	6
46	Computer Simulations of Interphases and Solute Transfer in Liquid and Size Exclusion Chromatography. ACS Symposium Series, 1999, , 67-81.	0.5	4
47	Comment on ion transit pathways and gating in ClC chloride channels. Proteins: Structure, Function and Bioinformatics, 2005, 62, 553-554.	2.6	4
48	Specific Ion Solvation and Pairing Effects in Glycerol Carbonate. Journal of Physical Chemistry B, 2021, 125, 13635-13643.	2.6	4
49	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
50	Investigating partitioning of freeversusmacrocycle bound guest into a model POPC lipid bilayer. RSC Advances, 2020, 10, 15148-15153.	3.6	2
51	Quantum Contributions to Free Energy Changes in Fluids. Springer Series in Chemical Physics, 2007, , 389-422.	0.2	2
52	Methods of Single-Step and Multistep Particle Switching in Simulations of Mixtures. The Journal of Physical Chemistry, 1996, 100, 16002-16005.	2.9	1
53	A real-space stochastic density matrix approach for density functional electronic structure. Physical Chemistry Chemical Physics, 2015, 17, 31472-31479.	2.8	1
54	Multiscale techniques for electrostatics and eigenvalue problems in real space. , 1999, , .		0

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55	Solving the SchrÃ¶dinger Equation on Real-Space Grids and with Random Walks. , 2011, , 271-311.		0
56	Tribute to Lawrence R. Pratt. Journal of Physical Chemistry B, 2021, 125, 4925-4927.	2.6	0