

Stefan M Kast

List of Publications by Year in descending order

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56
papers

1,481
citations

279798

23
h-index

330143

37
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59
all docs

59
docs citations

59
times ranked

1458
citing authors

#	ARTICLE	IF	CITATIONS
1	Binary Phases of Aliphatic N-Oxides and Water: A Force Field Development and Molecular Dynamics Simulation. <i>Journal of Physical Chemistry A</i> , 2003, 107, 5342-5351.	2.5	123
2	Overcoming EGFR G724S-mediated osimertinib resistance through unique binding characteristics of second-generation EGFR inhibitors. <i>Nature Communications</i> , 2018, 9, 4655.	12.8	107
3	Targeting Drug Resistance in EGFR with Covalent Inhibitors: A Structure-Based Design Approach. <i>Journal of Medicinal Chemistry</i> , 2015, 58, 6844-6863.	6.4	92
4	Design principles for high-pressure force fields: Aqueous TMAO solutions from ambient to kilobar pressures. <i>Journal of Chemical Physics</i> , 2016, 144, 144104.	3.0	79
5	Closed-form expressions of the chemical potential for integral equation closures with certain bridge functions. <i>Journal of Chemical Physics</i> , 2008, 129, 236101.	3.0	76
6	Quantum Chemistry in Solution by Combining 3D Integral Equation Theory with a Cluster Embedding Approach. <i>Journal of Physical Chemistry B</i> , 2008, 112, 4337-4343.	2.6	69
7	Drugging the catalytically inactive state of RET kinase in RET-rearranged tumors. <i>Science Translational Medicine</i> , 2017, 9, .	12.4	55
8	Signatures of Solvation Thermodynamics in Spectra of Intermolecular Vibrations. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 4467-4481.	5.3	52
9	Combinations of simulation and integral equation theory. <i>Physical Chemistry Chemical Physics</i> , 2001, 3, 5087-5092.	2.8	48
10	Toward Extreme Biophysics: Deciphering the Infrared Response of Biomolecular Solutions at High Pressures. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 9534-9538.	13.8	47
11	Evaluation of log $\hat{A}P$, pKa, and log $\hat{A}D$ predictions from the SAMPL7 blind challenge. <i>Journal of Computer-Aided Molecular Design</i> , 2021, 35, 771-802.	2.9	42
12	Molecular Dynamics Simulation of the Cytosolic Mouth in Kcv-Type Potassium Channels. <i>Biochemistry</i> , 2007, 46, 4826-4839.	2.5	40
13	Long Distance Interactions within the Potassium Channel Pore Are Revealed by Molecular Diversity of Viral Proteins. <i>Journal of Biological Chemistry</i> , 2004, 279, 28443-28449.	3.4	38
14	Chlorella virus ATCV-1 encodes a functional potassium channel of 82 amino acids. <i>Biochemical Journal</i> , 2009, 420, 295-305.	3.7	38
15	Model Development for the Viral Kcv Potassium Channel. <i>Biophysical Journal</i> , 2009, 96, 485-498.	0.5	35
16	Minimal art: Or why small viral K ⁺ channels are good tools for understanding basic structure and function relations. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2011, 1808, 580-588.	2.6	35
17	Prediction of tautomer ratios by embedded-cluster integral equation theory. <i>Journal of Computer-Aided Molecular Design</i> , 2010, 24, 343-353.	2.9	34
18	Viral potassium channels as a robust model system for studies of membrane-protein interaction. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2014, 1838, 1096-1103.	2.6	28

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19	The SAMPL5 challenge for embedded-cluster integral equation theory: solvation free energies, aqueous pK _a , and cyclohexane-water log D. <i>Journal of Computer-Aided Molecular Design</i> , 2016, 30, 1035-1044.	2.9	28
20	The SAMPL6 challenge on predicting aqueous pK _a values from EC-RISM theory. <i>Journal of Computer-Aided Molecular Design</i> , 2018, 32, 1151-1163.	2.9	28
21	Solvation Effects on Chemical Shifts by Embedded Cluster Integral Equation Theory. <i>Journal of Physical Chemistry A</i> , 2014, 118, 11620-11628.	2.5	26
22	3D RISM theory with fast reciprocal-space electrostatics. <i>Journal of Chemical Physics</i> , 2015, 142, 114107.	3.0	23
23	The Chemical Shift Baseline for High-Pressure NMR Spectra of Proteins. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 8757-8760.	13.8	23
24	Tautomeric Equilibria of Nucleobases in the Hachimoji Expanded Genetic Alphabet. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 2766-2777.	5.3	22
25	Free energies from integral equation theories: Enforcing path independence. <i>Physical Review E</i> , 2003, 67, 041203.	2.1	19
26	Integral equation theory for correcting truncation errors in molecular simulations. <i>Chemical Physics Letters</i> , 2003, 367, 398-404.	2.6	18
27	Three-Dimensional RISM Integral Equation Theory for Polarizable Solute Models. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 4718-4726.	5.3	18
28	Identification of Intrahelical Bifurcated H-Bonds as a New Type of Gate in K ⁺ Channels. <i>Journal of the American Chemical Society</i> , 2017, 139, 7494-7503.	13.7	17
29	Thermodynamic Characterization of Hydration Sites from Integral Equation-Derived Free Energy Densities: Application to Protein Binding Sites and Ligand Series. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 1652-1666.	5.4	17
30	Hybrid Integral Equation/Monte Carlo Approach to Complexation Thermodynamics. <i>Journal of Physical Chemistry B</i> , 2002, 106, 6289-6297.	2.6	16
31	The SAMPL6 challenge on predicting octanol-water partition coefficients from EC-RISM theory. <i>Journal of Computer-Aided Molecular Design</i> , 2020, 34, 453-461.	2.9	16
32	Chemically Stabilized DNA Barcodes for DNA-Encoded Chemistry. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 19744-19749.	13.8	15
33	Parametrization Strategy for the MolFESD Concept: Quantitative Surface Representation of Local Hydrophobicity. <i>Journal of Chemical Information and Computer Sciences</i> , 2003, 43, 237-247.	2.8	14
34	Pressure-dependent electronic structure calculations using integral equation-based solvation models. <i>Biophysical Chemistry</i> , 2020, 257, 106258.	2.8	14
35	Acidity in DMSO from the embedded cluster integral equation quantum solvation model. <i>Journal of Molecular Modeling</i> , 2014, 20, 2161.	1.8	13
36	The hpCADD NDDO Hamiltonian: Parametrization. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 1907-1922.	5.4	11

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37	A Joint Venture of Ab Initio Molecular Dynamics, Coupled Cluster Electronic Structure Methods, and Liquid-State Theory to Compute Accurate Isotropic Hyperfine Constants of Nitroxide Probes in Water. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 6366-6386.	5.3	11
38	Thermally induced polarizabilities and dipole moments of small tin clusters. <i>Journal of Chemical Physics</i> , 2012, 136, 134320.	3.0	10
39	Structure and thermodynamics of aqueous urea solutions from ambient to kilobar pressures: From thermodynamic modeling, experiments, and first principles simulations to an accurate force field description. <i>Biophysical Chemistry</i> , 2019, 254, 106260.	2.8	10
40	A minimalist model for ion partitioning and competition in a K ⁺ channel selectivity filter. <i>Journal of General Physiology</i> , 2011, 138, 371-373.	1.9	9
41	pKa calculations for tautomerizable and conformationally flexible molecules: partition function vs. state transition approach. <i>Journal of Molecular Modeling</i> , 2019, 25, 139.	1.8	9
42	Quantum-mechanical property prediction of solvated drug molecules: what have we learned from a decade of SAMPL blind prediction challenges?. <i>Journal of Computer-Aided Molecular Design</i> , 2021, 35, 453-472.	2.9	9
43	Hybrid Integral-Equation/Simulation Models: From Complexation Thermodynamics to Direct Free Energies. <i>ChemPhysChem</i> , 2004, 5, 449-455.	2.1	8
44	Addendum to "Free energies from integral equation theories: Enforcing path independence". <i>Physical Review E</i> , 2006, 73, 012201.	2.1	5
45	Bridge function of the repulsive Weeks-Chandler-Andersen (WCA) fluid. <i>Chemical Physics Letters</i> , 2014, 591, 237-242.	2.6	5
46	Structure and thermodynamics of nondipolar molecular liquids and solutions from integral equation theory. <i>Molecular Physics</i> , 2016, 114, 2461-2476.	1.7	5
47	SAMPL7 physical property prediction from EC-RISM theory. <i>Journal of Computer-Aided Molecular Design</i> , 2021, 35, 933-941.	2.9	5
48	Toward Extreme Biophysics: Deciphering the Infrared Response of Biomolecular Solutions at High Pressures. <i>Angewandte Chemie</i> , 2016, 128, 9686-9690.	2.0	4
49	Fast prediction of hydration free energies from molecular interaction fields. <i>Journal of Molecular Graphics and Modelling</i> , 2001, 20, 123-131.	2.4	3
50	Die Basislinie der chemischen Verschiebung in Hochdruck-NMR-Spektren von Proteinen. <i>Angewandte Chemie</i> , 2016, 128, 8900-8904.	2.0	3
51	Communication: An exact bound on the bridge function in integral equation theories. <i>Journal of Chemical Physics</i> , 2012, 137, 171102.	3.0	2
52	11th German Conference on Chemoinformatics (GCC 2015). <i>Journal of Cheminformatics</i> , 2016, 8, 18.	6.1	1
53	High pressure response of ¹ H NMR chemical shifts of purine nucleotides. <i>Biophysical Chemistry</i> , 2019, 254, 106261.	2.8	1
54	Asymmetric Interplay Between K ⁺ and Blocker and Atomistic Parameters From Physiological Experiments Quantify K ⁺ Channel Blocker Release. <i>Frontiers in Physiology</i> , 2021, 12, 737834.	2.8	1

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55	Investigations Into Chemically Stabilized Four-Letter DNA for DNA-Encoded Chemistry. <i>Frontiers in Chemistry</i> , 0, 10, .	3.6	1
56	Chemisch stabilisierte DNAâ€Codes fÃ¼r DNAâ€kodierte Chemie. <i>Angewandte Chemie</i> , 2021, 133, 19897-19902.2.0		0