Stefan Boresch

List of Publications by Year
in descending order

56 papers	10,151 citations	145106 33 h-index	169272 56 g-index
56 all docs	56 docs citations	56 times ranked	13461 citing authors

#	Article	IF	Citations
1	Optimizing the Calculation of Free Energy Differences in Nonequilibrium Work SQM/MM Switching Simulations. Journal of Physical Chemistry B, 2022, 126, 2798-2811.	1.2	5
2	Alchemical free energy simulations without speed limits. A generic framework to calculate free energy differences independent of the underlying molecular dynamics program. Journal of Computational Chemistry, 2022, , .	1.5	5
3	Dummy Atoms in Alchemical Free Energy Calculations. Journal of Chemical Theory and Computation, 2021, 17, 4403-4419.	2.3	20
4	Polarizable molecular dynamics simulations of ionic liquids: Influence of temperature control. Journal of Chemical Physics, 2020, 152, 094105.	1.2	12
5	Use of Interaction Energies in QM/MM Free Energy Simulations. Journal of Chemical Theory and Computation, 2019, 15, 4632-4645.	2.3	21
6	The Good, the Bad, and the Ugly: â€œHiPenâ€ a New Dataset for Validating (S)QM/MM Free Energy Simulations. Molecules, 2019, 24, 681.	1.7	9
7	Accelerating QM/MM Free Energy Computations via Intramolecular Force Matching. Journal of Chemical Theory and Computation, 2018, 14, 6327-6335.	2.3	40
8	SAR-Guided Scoring Function and Mutational Validation Reveal the Binding Mode of CGS-8216 at the Î±1+/Î²2â€“ Benzodiazepine Site. Journal of Chemical Information and Modeling, 2018, 58, 1682-1696.	2.5	5
9	Common Hits Approach: Combining Pharmacophore Modeling and Molecular Dynamics Simulations. Journal of Chemical Information and Modeling, 2017, 57, 365-385.	2.5	59
10	Computing converged free energy differences between levels of theory via nonequilibrium work methods: Challenges and opportunities. Journal of Computational Chemistry, 2017, 38, 1376-1388.	1.5	28
11	Convergence of single-step free energy perturbation. Molecular Physics, 2017, 115, 1200-1213.	0.8	46
12	Methods for Efficiently and Accurately Computing Quantum Mechanical Free Energies for Enzyme Catalysis. Methods in Enzymology, 2016, 577, 75-104.	0.4	6
13	Evaluating the stability of pharmacophore features using molecular dynamics simulations. Biochemical and Biophysical Research Communications, 2016, 470, 685-689.	1.0	26
14	Comparing pharmacophore models derived from crystal structures and from molecular dynamics simulations. Monatshefte FÃ¼r Chemie, 2016, 147, 553-563.	0.9	15
15	Use of Nonequilibrium Work Methods to Compute Free Energy Differences Between Molecular Mechanical and Quantum Mechanical Representations of Molecular Systems. Journal of Physical Chemistry Letters, 2015, 6, 4850-4856.	2.1	55
16	Efficiently computing pathway free energies: New approaches based on chain-of-replica and Non-Boltzmann Bennett reweighting schemes. Biochimica Et Biophysica Acta - General Subjects, 2015, 1850, 944-953.	1.1	28
17	Web-Based Computational Chemistry Education with CHARMMing I: Lessons and Tutorial. PLoS Computational Biology, 2014, 10, e1003719.	1.5	14
18	Transport and dielectric properties of water and the influence of coarse-graining: Comparing BMW, SPC/E, and TIP3P models. Journal of Chemical Physics, 2014, 140, 064107.	1.2	55

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19	Multiscale Free Energy Simulations: An Efficient Method for Connecting Classical MD Simulations to QM or QM/MM Free Energies Using Non-Boltzmann Bennett Reweighting Schemes. Journal of Chemical Theory and Computation, 2014, 10, 1406-1419.	2.3	111
20	Comparison of thermodynamic integration and Bennett acceptance ratio for calculating relative proteinâ€ligand binding free energies. Journal of Computational Chemistry, 2013, 34, 1024-1034.	1.5	63
21	Absolute Hydration Free Energies of Blocked Amino Acids: Implications for Protein Solvation and Stability. Biophysical Journal, 2013, 104, 453-462.	0.2	52
22	Enhanced Sampling in Free Energy Calculations: Combining SGLD with the Bennettâ€™s Acceptance Ratio and Enveloping Distribution Sampling Methods. Journal of Chemical Theory and Computation, 2012, 8, 3650-3662.	2.3	18
23	Nonâ€Boltzmann sampling and Bennett's acceptance ratio method: How to profit from bending the rules. Journal of Computational Chemistry, 2011, 32, 1082-1090.	1.5	63
24	Efficiency of alchemical free energy simulations. II. Improvements for thermodynamic integration. Journal of Computational Chemistry, 2011, 32, 1320-1333.	1.5	90
25	Efficiency of alchemical free energy simulations. I. A practical comparison of the exponential formula, thermodynamic integration, and Bennett's acceptance ratio method. Journal of Computational Chemistry, 2011, 32, 1303-1319.	1.5	94
26	Avoiding the van der Waals endpoint problem using serial atomic insertion. Journal of Computational Chemistry, 2011, 32, 2449-2458.	1.5	23
27	Unorthodox uses of Bennett's acceptance ratio method. Journal of Computational Chemistry, 2009, 30, 1712-1718.	1.5	38
28	CHARMM: The biomolecular simulation program. Journal of Computational Chemistry, 2009, 30, 1545-1614.	1.5	7,077
29	Hydration Free Energies of Amino Acids: Why Side Chain Analog Data Are Not Enough. Journal of Physical Chemistry B, 2009, 113, 8967-8974.	1.2	57
30	Single molecule pulling with large time steps. Physical Review E, 2007, 75, 061106.	0.8	23
31	A molecular dynamics study of WPD-loop flexibility in PTP1B. Biochemical and Biophysical Research Communications, 2007, 356, 1011-1016.	1.0	65
32	A targeted molecular dynamics study of WPD loop movement in PTP1B. Biochemical and Biophysical Research Communications, 2006, 345, 1161-1166.	1.0	45
33	Simulation studies of the protein-water interface. II. Properties at the mesoscopic resolution. Journal of Chemical Physics, 2006, 124, 234908.	1.2	39
34	Simulation studies of the protein-water interface. I. Properties at the molecular resolution. Journal of Chemical Physics, 2006, 124, 234907.	1.2	75
35	Alchemical free energy calculations and multiple conformational substates. Journal of Chemical Physics, 2005, 122, 084109.	1.2	56
36	Comparative Models of GABAA Receptor Extracellular and Transmembrane Domains: Important Insights in Pharmacology and Function. Molecular Pharmacology, 2005, 68, 1291-1300.	1.0	132

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37	Unexpected Relative Aqueous Solubilities of a Phosphotyrosine Analogue and Two Phosphonate Derivatives. Journal of the American Chemical Society, 2005, 127, 4640-4648.	6.6	11
38	A molecular dynamics study of the dielectric properties of aqueous solutions of alanine and alanine dipeptide. Journal of Chemical Physics, 2004, 120, 3333-3347.	1.2	34
39	Comparative modeling of GABAA receptors: limits, insights, future developments. Neuroscience, 2003, 119, 933-943.	1.1	140
40	Absolute Binding Free Energies:Â A Quantitative Approach for Their Calculation. Journal of Physical Chemistry B, 2003, 107, 9535-9551.	1.2	449
41	The Role of Bonded Energy Terms in Free Energy Simulations - Insights from Analytical Results. Molecular Simulation, 2002, 28, 13-37.	0.9	32
42	Comments on â€œAnomalous Dielectric Relaxation of Aqueous Protein Solutionsâ€•by Nilashis Nandi and Biman Bagchi (J. Phys. Chem. A1998,102, 8217). Journal of Physical Chemistry A, 2001, 105, 5507-5508.	1.1	3
43	Dielectric spectroscopy in aqueous solutions of oligosaccharides: Experiment meets simulation. Journal of Chemical Physics, 2001, 115, 1463-1472.	1.2	52
44	The dielectric self-consistent field method. II. Application to the study of finite range effects. Journal of Chemical Physics, 2001, 115, 10793-10807.	1.2	24
45	The dielectric self-consistent field method. I. Highways, byways, and illustrative results. Journal of Chemical Physics, 2001, 115, 10780-10792.	1.2	18
46	Influence of the treatment of electrostatic interactions on the results of free energy calculations of dipolar systems. Journal of Chemical Physics, 2000, 112, 6953-6955.	1.2	20
47	Dielectric properties of glucose and maltose solutions. Journal of Chemical Physics, 2000, 112, 9810-9821.	1.2	42
48	Towards a better description and understanding of biomolecular solvation. Biophysical Chemistry, 1999, 78, 43-68.	1.5	43
49	Rationalizing the effects of modified electrostatic interactions in computer simulations: The dielectric self-consistent field method. Journal of Chemical Physics, 1999, 111, 8271-8274.	1.2	22
50	The Role of Bonded Terms in Free Energy Simulations:â€‰ 1. Theoretical Analysis. Journal of Physical Chemistry A, 1999, 103, 103-118.	1.1	116
51	The Role of Bonded Terms in Free Energy Simulations. 2. Calculation of Their Influence on Free Energy Differences of Solvation. Journal of Physical Chemistry A, 1999, 103, 119-136.	1.1	80
52	Rationalization of the dielectric properties of common three-site water models in terms of their force field parameters. Journal of Chemical Physics, 1998, 109, 4927-4937.	1.2	128
53	Presumed versus real artifacts of the Ewald summation technique: The importance of dielectric boundary conditions. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1997, 101, 1019-1029.	0.9	46
54	The Jacobian factor in free energy simulations. Journal of Chemical Physics, 1996, 105, 5145-5154.	1.2	61

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55	The Meaning of Component Analysis: Decomposition of the Free Energy in Terms of Specific Interactions. Journal of Molecular Biology, 1995, 254, 801-807.	2.0	139
56	Free energy simulations: The meaning of the individual contributions from a component analysis. Proteins: Structure, Function and Bioinformatics, 1994, 20, 25-33.	1.5	121