

# Gerhard König

## List of Publications by Year in descending order

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Version: 2024-02-01

41  
papers

1,121  
citations

448610

19  
h-index

466096

32  
g-index

41  
all docs

41  
docs citations

41  
times ranked

1139  
citing authors

#	ARTICLE	IF	CITATIONS
1	Comparative Performance of PETase as a Function of Reaction Conditions, Substrate Properties, and Product Accumulation. <i>ChemSusChem</i> , 2022, 15, .	3.6	42
2	Mechanistic details of the actinobacterial lyase-catalyzed degradation reaction of 2-hydroxyisobutyryl-CoA. <i>Journal of Biological Chemistry</i> , 2022, 298, 101522.	1.6	2
3	Relative free-energy calculations for scaffold hopping-type transformations with an automated RE-EDS sampling procedure. <i>Journal of Computer-Aided Molecular Design</i> , 2022, 36, 117-130.	1.3	10
4	Ensembler: A Simple Package for Fast Prototyping and Teaching Molecular Simulations. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 560-564.	2.5	4
5	Effect of Flexibility, Lipophilicity, and the Location of Polar Residues on the Passive Membrane Permeability of a Series of Cyclic Decapeptides. <i>Journal of Medicinal Chemistry</i> , 2021, 64, 12761-12773.	2.9	22
6	Efficient Alchemical Intermediate States in Free Energy Calculations Using $\hat{\nu}$ -Enveloping Distribution Sampling. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 5805-5815.	2.3	8
7	1-Butanol: An Ecologically and Economically Viable Extraction Solvent for Isolating Polar Products from Aqueous Solutions. <i>European Journal of Organic Chemistry</i> , 2021, 2021, 6224-6228.	1.2	5
8	Rational prioritization strategy allows the design of macrolide derivatives that overcome antibiotic resistance. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, e2113632118.	3.3	7
9	An Alternative to Conventional $\hat{\nu}$ -Intermediate States in Alchemical Free Energy Calculations: $\hat{\nu}$ -Enveloping Distribution Sampling. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 5407-5423.	2.5	18
10	On the faithfulness of molecular mechanics representations of proteins towards quantum-mechanical energy surfaces. <i>Interface Focus</i> , 2020, 10, 20190121.	1.5	13
11	Overcoming Orthogonal Barriers in Alchemical Free Energy Calculations: On the Relative Merits of $\hat{\nu}$ -Variations, $\hat{\nu}$ -Extrapolations, and Biasing. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 1630-1645.	2.3	20
12	A Comparison of QM/MM Simulations with and without the Drude Oscillator Model Based on Hydration Free Energies of Simple Solutes. <i>Molecules</i> , 2018, 23, 2695.	1.7	29
13	On the convergence of multi-scale free energy simulations. <i>Molecular Simulation</i> , 2018, 44, 1062-1081.	0.9	42
14	1-Butanol as a Solvent for Efficient Extraction of Polar Compounds from Aqueous Medium: Theoretical and Practical Aspects. <i>Journal of Physical Chemistry B</i> , 2018, 122, 6975-6988.	1.2	24
15	An Estimation of Hybrid Quantum Mechanical Molecular Mechanical Polarization Energies for Small Molecules Using Polarizable Force-Field Approaches. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 679-695.	2.3	19
16	Absolute binding free energies for octa-acids and guests in SAMPL5. <i>Journal of Computer-Aided Molecular Design</i> , 2017, 31, 107-118.	1.3	16
17	Absolute binding free energy calculations of CBClip host-guest systems in the SAMPL5 blind challenge. <i>Journal of Computer-Aided Molecular Design</i> , 2017, 31, 71-85.	1.3	13
18	Blind prediction of distribution in the SAMPL5 challenge with QM based protomer and pK a corrections. <i>Journal of Computer-Aided Molecular Design</i> , 2016, 30, 1087-1100.	1.3	27

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19	An efficient protocol for obtaining accurate hydration free energies using quantum chemistry and reweighting from molecular dynamics simulations. <i>Bioorganic and Medicinal Chemistry</i> , 2016, 24, 4988-4997.	1.4	15
20	Calculating distribution coefficients based on multi-scale free energy simulations: an evaluation of MM and QM/MM explicit solvent simulations of water-cyclohexane transfer in the SAMPL5 challenge. <i>Journal of Computer-Aided Molecular Design</i> , 2016, 30, 989-1006.	1.3	24
21	Calculations of Solvation Free Energy through Energy Reweighting from Molecular Mechanics to Quantum Mechanics. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 499-511.	2.3	78
22	Comparison of Methods To Reweight from Classical Molecular Simulations to QM/MM Potentials. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 1466-1480.	2.3	42
23	Computation of Hydration Free Energies Using the Multiple Environment Single System Quantum Mechanical/Molecular Mechanical Method. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 332-344.	2.3	42
24	Multiple Environment Single System Quantum Mechanical/Molecular Mechanical (MESS-QM/MM) Calculations. 1. Estimation of Polarization Energies. <i>Journal of Physical Chemistry A</i> , 2015, 119, 1511-1523.	1.1	23
25	Quantum Mechanical Molecular Mechanical Calculations using AMOEBA Force Fields. <i>Biophysical Journal</i> , 2015, 108, 158a.	0.2	1
26	Correcting for the free energy costs of bond or angle constraints in molecular dynamics simulations. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2015, 1850, 932-943.	1.1	38
27	Predicting hydration free energies with a hybrid QM/MM approach: an evaluation of implicit and explicit solvation models in SAMPL4. <i>Journal of Computer-Aided Molecular Design</i> , 2014, 28, 245-257.	1.3	59
28	Computing the Free Energy along a Reaction Coordinate Using Rigid Body Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 4198-4207.	2.3	14
29	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. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 1406-1419.	2.3	111
30	Simulation and the Problem of Simplification. <i>Philosophy and Technology</i> , 2013, 26, 81-91.	2.6	1
31	Absolute Hydration Free Energies of Blocked Amino Acids: Implications for Protein Solvation and Stability. <i>Biophysical Journal</i> , 2013, 104, 453-462.	0.2	52
32	Enhanced Sampling in Free Energy Calculations: Combining SGLD with the Bennett's Acceptance Ratio and Enveloping Distribution Sampling Methods. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 3650-3662.	2.3	18
33	Predicting binding affinities of host-guest systems in the SAMPL3 blind challenge: the performance of relative free energy calculations. <i>Journal of Computer-Aided Molecular Design</i> , 2012, 26, 543-550.	1.3	27
34	Computing eigenvectors of block tridiagonal matrices based on twisted block factorizations. <i>Journal of Computational and Applied Mathematics</i> , 2012, 236, 3696-3703.	1.1	6
35	Non-Boltzmann sampling and Bennett's acceptance ratio method: How to profit from bending the rules. <i>Journal of Computational Chemistry</i> , 2011, 32, 1082-1090.	1.5	63
36	On twisted factorizations of block tridiagonal matrices. <i>Procedia Computer Science</i> , 2010, 1, 279-287.	1.2	2

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37	Unorthodox uses of Bennett's acceptance ratio method. Journal of Computational Chemistry, 2009, 30, 1712-1718.	1.5	38
38	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
39	Hydrophobic moments as physicochemical descriptors in structure-activity relationship studies of P-glycoprotein inhibitors. Monatshefte für Chemie, 2008, 139, 401-405.	0.9	7
40	Synthesis and structure activity relationships of novel small molecule cathepsin D inhibitors. Bioorganic and Medicinal Chemistry Letters, 1999, 9, 2531-2536.	1.0	79
41	Testing and Optimizing the Drude Polarizable Force Field for Blocked Amino Acids Based on High-Level Quantum-Mechanical Energy Surfaces. Journal of Computational Biophysics and Chemistry, 0, , 1-9.	1.0	3