Michael Schauperl

List of Publications by Year
in descending order

37 papers	917 citations	516561 16 h-index	477173 29 g-index
54 all docs	54 docs citations	54 times ranked	1367 citing authors

#	Article	IF	Citations
1	Ice nucleation by water-soluble macromolecules. Atmospheric Chemistry and Physics, 2015, 15, 4077-4091.	1.9	198
2	Non-bonded force field model with advanced restrained electrostatic potential charges (RESP2). Communications Chemistry, 2020, 3, .	2.0	98
3	Enthalpic and Entropic Contributions to Hydrophobicity. Journal of Chemical Theory and Computation, 2016, 12, 4600-4610.	2.3	68
4	Perspectives on the Future of Ice Nucleation Research: Research Needs and Unanswered Questions Identified from Two International Workshops. Atmosphere, 2017, 8, 138.	1.0	56
5	Coilâ€“Globule Transition Thermodynamics of Poly(N-isopropylacrylamide). Journal of Physical Chemistry B, 2019, 123, 8838-8847.	1.2	45
6	Solvation Free Energy as a Measure of Hydrophobicity: Application to Serine Protease Binding Interfaces. Journal of Chemical Theory and Computation, 2019, 15, 5872-5882.	2.3	42
7	New High-Pressure Gallium Borate Ga₂B₃O₇(OH) with Photocatalytic Activity. Inorganic Chemistry, 2016, 55, 676-681.	1.9	36
8	AI-Based Protein Structure Prediction in Drug Discovery: Impacts and Challenges. Journal of Chemical Information and Modeling, 2022, 62, 3142-3156.	2.5	36
9	Highâ€Pressure Synthesis of Cd(NH₃)₂[B₃O₅(NH₃)]₂: Pioneering the Way to the Substance Class of Ammine Borates. Angewandte Chemie - International Edition, 2015, 54, 6360-6363.	7.2	33
10	CaB₂S₄O₁₆: A Borosulfate Exhibiting a New Structure Type with Phyllosilicate Analogue Topology. Chemistry - A European Journal, 2017, 23, 16773-16781.	1.7	25
11	Characterizing Protease Specificity: How Many Substrates Do We Need?. PLoS ONE, 2015, 10, e0142658.	1.1	25
12	Balance between hydration enthalpy and entropy is important for ice binding surfaces in Antifreeze Proteins. Scientific Reports, 2017, 7, 11901.	1.6	21
13	Probing the Structural and Binding Mechanism Heterogeneity of Molecularly Imprinted Polymers. Journal of Physical Chemistry B, 2015, 119, 563-571.	1.2	20
14	Binding Pose Flip Explained via Enthalpic and Entropic Contributions. Journal of Chemical Information and Modeling, 2017, 57, 345-354.	2.5	20
15	Ag[B(SO₄)₂] â€“ Synthesis, Crystal Structure, and Characterization of the First Preciousâ€Metal Borosulfate. European Journal of Inorganic Chemistry, 2017, 2017, 3981-3989.	1.0	19
16	Quantum Chemical Microsolvation by Automated Water Placement. Molecules, 2021, 26, 1793.	1.7	18
17	Data-Driven Mapping of Gas-Phase Quantum Calculations to General Force Field Lennard-Jones Parameters. Journal of Chemical Theory and Computation, 2020, 16, 1115-1127.	2.3	15
18	Macrocycle Cell Permeability Measured by Solvation Free Energies in Polar and Apolar Environments. Journal of Chemical Information and Modeling, 2020, 60, 3508-3517.	2.5	15

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19	Electrostatic recognition in substrate binding to serine proteases. Journal of Molecular Recognition, 2018, 31, e2727.	1.1	13
20	Benchmarking Electronic Structure Methods for Accurate Fixed-Charge Electrostatic Models. Journal of Chemical Information and Modeling, 2020, 60, 249-258.	2.5	12
21	Orthorhombic HPâ€REOF (RE = Pr, Nd, Sm â€“ Gd) â€“ Highâ€Pressure Syntheses and Singleâ€Crystal Structures (RE = Nd, Sm, Eu). Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2016, 642, 1134-1142.	0.6	11
22	Hydration of Aromatic Heterocycles as an Adversary of Ï€-Stacking. Journal of Chemical Information and Modeling, 2019, 59, 4209-4219.	2.5	11
23	Solvation Thermodynamics in Different Solvents: Waterâ€“Chloroform Partition Coefficients from Grid Inhomogeneous Solvation Theory. Journal of Chemical Information and Modeling, 2020, 60, 3843-3853.	2.5	11
24	Structure, Thermal Behavior, and Vibrational Spectroscopy of the Silver Borate AgB₃O₅. European Journal of Inorganic Chemistry, 2015, 2015, 527-533.	1.0	10
25	STACKED â€“ <u>S</u>olvation <u>T</u>heory of <u>A</u>romatic <u>C</u>omplexes as <u>K</u>ey for <u>E</u>stimating <u>D</u>rug Binding. Journal of Chemical Information and Modeling, 2020, 60, 2304-2313.	2.5	10
26	Performance of DFT functionals for properties of small molecules containing beryllium, tungsten and hydrogen. Nuclear Materials and Energy, 2020, 22, 100731.	0.6	8
27	High-pressure synthesis and crystal structure of In₃B₅O₁₂. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2017, 72, 69-76.	0.3	6
28	Data-driven analysis of the number of Lennardâ€“Jones types needed in a force field. Communications Chemistry, 2020, 3, .	2.0	6
29	Quantitative Correlation of Conformational Binding Enthalpy with Substrate Specificity of Serine Proteases. Journal of Physical Chemistry B, 2016, 120, 299-308.	1.2	5
30	Protease Inhibitors in View of Peptide Substrate Databases. Journal of Chemical Information and Modeling, 2016, 56, 1228-1235.	2.5	4
31	Synthesis and characterization of a disordered variant of KB₅O₇(OH)₂. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2015, 70, 649-658.	0.3	2
32	Hydration thermodynamics of cytosolic phospholipase A2 GIVA predict its membrane-associated parts and its highly hydrated binding site. Journal of Biomolecular Structure and Dynamics, 2021, 39, 953-959.	2.0	1
33	Conformational Shifts of Stacked Heteroaromatics: Vacuum vs. Water Studied by Machine Learning. Frontiers in Chemistry, 2021, 9, 641610.	1.8	1
34	Innentitelbild: Hochdrucksynthese von Cd(NH3)2[B3O5(NH3)]2: ein grundlegender Weg in die Substanzklasse der Amminborate (Angew. Chem. 21/2015). Angewandte Chemie, 2015, 127, 6168-6168.	1.6	0
35	Front Cover: Ag[B(SO4)2] - Synthesis, Crystal Structure, and Characterization of the First Precious-Metal Borosulfate (Eur. J. Inorg. Chem. 34/2017). European Journal of Inorganic Chemistry, 2017, 2017, 3979-3979.	1.0	0
36	Ag[B(SO4)2] - Synthesis, Crystal Structure, and Characterization of the First Precious-Metal Borosulfate. European Journal of Inorganic Chemistry, 2017, 2017, 3980-3980.	1.0	0

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37	Frontispiece: CaB₂S₄O₁₆: A Borosulfate Exhibiting a New Structure Type with Phyllosilicate Analogue Topology. Chemistry - A European Journal, 2017, 23, .	1.7	0