# Michael Schauperl

List of Publications by Year
in descending order



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|---|---|---|---|
| 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 | AI-Based Protein Structure Prediction in Drug Discovery: Impacts and Challenges. Journal of Chemical Information and Modeling, 2022, 62, 3142-3156. | 2.5 | 36 |
| 2 | 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 |
| 3 | Conformational Shifts of Stacked Heteroaromatics: Vacuum vs. Water Studied by Machine Learning. Frontiers in Chemistry, 2021, 9, 641610. | 1.8 | 1 |
| 4 | Quantum Chemical Microsolvation by Automated Water Placement. Molecules, 2021, 26, 1793. | 1.7 | 18 |
| 5 | 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 |
| 6 | Benchmarking Electronic Structure Methods for Accurate Fixed-Charge Electrostatic Models. Journal of Chemical Information and Modeling, 2020, 60, 249-258. | 2.5 | 12 |
| 7 | 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 |
| 8 | Data-driven analysis of the number of Lennardâ€“Jones types needed in a force field. Communications Chemistry, 2020, 3, . | 2.0 | 6 |
| 9 | 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 |
| 10 | 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 |
| 11 | Performance of DFT functionals for properties of small molecules containing beryllium, tungsten and hydrogen. Nuclear Materials and Energy, 2020, 22, 100731. | 0.6 | 8 |
| 12 | Non-bonded force field model with advanced restrained electrostatic potential charges (RESP2). Communications Chemistry, 2020, 3, . | 2.0 | 98 |
| 13 | 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 |
| 14 | Hydration of Aromatic Heterocycles as an Adversary of Ï€-Stacking. Journal of Chemical Information and Modeling, 2019, 59, 4209-4219. | 2.5 | 11 |
| 15 | Coilâ€“Globule Transition Thermodynamics of Poly(N-isopropylacrylamide). Journal of Physical Chemistry B, 2019, 123, 8838-8847. | 1.2 | 45 |
| 16 | Electrostatic recognition in substrate binding to serine proteases. Journal of Molecular Recognition, 2018, 31, e2727. | 1.1 | 13 |
| 17 | High-pressure synthesis and crystal structure of In<sub>3</sub>B<sub>5</sub>O<sub>12</sub>. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2017, 72, 69-76. | 0.3 | 6 |
| 18 | Binding Pose Flip Explained via Enthalpic and Entropic Contributions. Journal of Chemical Information and Modeling, 2017, 57, 345-354. | 2.5 | 20 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | Ag[B(SO<sub>4</sub>)<sub>2</sub>] â€“ Synthesis, Crystal Structure, and Characterization of the First Preciousâ€Metal Borosulfate. European Journal of Inorganic Chemistry, 2017, 2017, 3981-3989. | 1.0 | 19 |
| 20 | CaB<sub>2</sub>S<sub>4</sub>O<sub>16</sub>: A Borosulfate Exhibiting a New Structure Type with Phyllosilicate Analogue Topology. Chemistry - A European Journal, 2017, 23, 16773-16781. | 1.7 | 25 |
| 21 | Balance between hydration enthalpy and entropy is important for ice binding surfaces in Antifreeze Proteins. Scientific Reports, 2017, 7, 11901. | 1.6 | 21 |
| 22 | 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 |
| 23 | 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 |
| 24 | Frontispiece: CaB<sub>2</sub>S<sub>4</sub>O<sub>16</sub>: A Borosulfate Exhibiting a New Structure Type with Phyllosilicate Analogue Topology. Chemistry - A European Journal, 2017, 23, . | 1.7 | 0 |
| 25 | 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 |
| 26 | 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 |
| 27 | Enthalpic and Entropic Contributions to Hydrophobicity. Journal of Chemical Theory and Computation, 2016, 12, 4600-4610. | 2.3 | 68 |
| 28 | Protease Inhibitors in View of Peptide Substrate Databases. Journal of Chemical Information and Modeling, 2016, 56, 1228-1235. | 2.5 | 4 |
| 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 | New High-Pressure Gallium Borate Ga<sub>2</sub>B<sub>3</sub>O<sub>7</sub>(OH) with Photocatalytic Activity. Inorganic Chemistry, 2016, 55, 676-681. | 1.9 | 36 |
| 31 | 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 |
| 32 | Highâ€Pressure Synthesis of Cd(NH<sub>3</sub>)<sub>2</sub>[B<sub>3</sub>O<sub>5</sub>(NH<sub>3</sub>)]<sub>2</sub>: Pioneering the Way to the Substance Class of Ammine Borates. Angewandte Chemie - International Edition, 2015, 54, 6360-6363. | 7.2 | 33 |
| 33 | Ice nucleation by water-soluble macromolecules. Atmospheric Chemistry and Physics, 2015, 15, 4077-4091. | 1.9 | 198 |
| 34 | Probing the Structural and Binding Mechanism Heterogeneity of Molecularly Imprinted Polymers. Journal of Physical Chemistry B, 2015, 119, 563-571. | 1.2 | 20 |
| 35 | Structure, Thermal Behavior, and Vibrational Spectroscopy of the Silver Borate AgB<sub>3</sub>O<sub>5</sub>. European Journal of Inorganic Chemistry, 2015, 2015, 527-533. | 1.0 | 10 |
| 36 | Synthesis and characterization of a disordered variant of KB<sub>5</sub>O<sub>7</sub>(OH)<sub>2</sub>. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2015, 70, 649-658. | 0.3 | 2 |

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| 37 | Characterizing Protease Specificity: How Many Substrates Do We Need?. PLoS ONE, 2015, 10, e0142658. | 1.1 | 25 |