# Maximilian Scheurer

List of Publications by Year
in descending order



| 19 | 1,797 | 759233 12 | 794594 19 |
|---|---|---|---|
| papers | citations | h-index | g-index |

| 33 | 33 | 33 | 1511 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | A long-lived fluorenyl cation: efficiency booster for uncaging and photobase properties. Physical Chemistry Chemical Physics, 2022, 24, 5294-5300. | 2.8 | 2 |
| 2 | Modeling Molecules under Pressure with Gaussian Potentials. Journal of Chemical Theory and Computation, 2021, 17, 583-597. | 5.3 | 17 |
| 3 | Selective Modification for Redâ€Shifted Excitability: A Small Change in Structure, a Huge Change in Photochemistry. Chemistry - A European Journal, 2021, 27, 2212-2218. | 3.3 | 11 |
| 4 | Gator: A Pythonâ€driven program for spectroscopy simulations using correlated wave functions. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1528. | 14.6 | 16 |
| 5 | Efficient Open-Source Implementations of Linear-Scaling Polarizable Embedding: Use Octrees to Save the Trees. Journal of Chemical Theory and Computation, 2021, 17, 3445-3454. | 5.3 | 7 |
| 6 | Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801. | 3.0 | 518 |
| 7 | Rethinking Uncaging: A New Antiaromatic Photocage Driven by a Gain of Resonance Energy. Chemistry - A European Journal, 2021, 27, 14121-14127. | 3.3 | 7 |
| 8 | Quantum Chemistry Common Driver and Databases (QCDB) and Quantum Chemistry Engine (QCE<scp>ngine</scp>): Automation and interoperability among computational chemistry programs. Journal of Chemical Physics, 2021, 155, 204801. | 3.0 | 15 |
| 9 | adcc: A versatile toolkit for rapid development of algebraicâ€diagrammatic construction methods. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1462. | 14.6 | 38 |
| 10 | Recent developments in the P<scp>y</scp>SCF program package. Journal of Chemical Physics, 2020, 153, 024109. | 3.0 | 388 |
| 11 | Complex excited state polarizabilities in the ADC/ISR framework. Journal of Chemical Physics, 2020, 153, 074112. | 3.0 | 9 |
| 12 | P<scp>SI4</scp> 1.4: Open-source software for high-throughput quantum chemistry. Journal of Chemical Physics, 2020, 152, 184108. | 3.0 | 440 |
| 13 | The rupture mechanism of rubredoxin is more complex than previously thought. Chemical Science, 2020, 11, 6036-6044. | 7.4 | 1 |
| 14 | VeloxChem: A Pythonâ€driven densityâ€functional theory program for spectroscopy simulations in highâ€performance computing environments. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1457. | 14.6 | 34 |
| 15 | CPPE: An Open-Source C++ and Python Library for Polarizable Embedding. Journal of Chemical Theory and Computation, 2019, 15, 6154-6163. | 5.3 | 20 |
| 16 | PyContact: Rapid, Customizable, and Visual Analysis of Noncovalent Interactions in MD Simulations. Biophysical Journal, 2018, 114, 577-583. | 0.5 | 80 |
| 17 | NAMD goes quantum: an integrative suite for hybrid simulations. Nature Methods, 2018, 15, 351-354. | 19.0 | 149 |
| 18 | Polarizable Embedding Combined with the Algebraic Diagrammatic Construction: Tackling Excited States in Biomolecular Systems. Journal of Chemical Theory and Computation, 2018, 14, 4870-4883. | 5.3 | 26 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | Molecular Mechanism of Flavin Photoprotection by Archaeal Dodecin: Photoinduced Electron Transfer and Mg<sup>2+</sup>-Promoted Proton Transfer. Journal of Physical Chemistry B, 2017, 121, 10457-10466. | 2.6 | 7 |