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	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
2	P<scp>SI4</scp> 1.4: Open-source software for high-throughput quantum chemistry. Journal of Chemical Physics, 2020, 152, 184108.	3.0	440
3	Recent developments in the P<scp>y</scp>SCF program package. Journal of Chemical Physics, 2020, 153, 024109.	3.0	388
4	NAMD goes quantum: an integrative suite for hybrid simulations. Nature Methods, 2018, 15, 351-354.	19.0	149
5	PyContact: Rapid, Customizable, and Visual Analysis of Noncovalent Interactions in MD Simulations. Biophysical Journal, 2018, 114, 577-583.	0.5	80
6	adcc: A versatile toolkit for rapid development of algebraicâ€diagrammatic construction methods. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1462.	14.6	38
7	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
8	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
9	CPPE: An Open-Source C++ and Python Library for Polarizable Embedding. Journal of Chemical Theory and Computation, 2019, 15, 6154-6163.	5.3	20
10	Modeling Molecules under Pressure with Gaussian Potentials. Journal of Chemical Theory and Computation, 2021, 17, 583-597.	5.3	17
11	Gator: A Pythonâ€driven program for spectroscopy simulations using correlated wave functions. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1528.	14.6	16
12	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
13	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
14	Complex excited state polarizabilities in the ADC/ISR framework. Journal of Chemical Physics, 2020, 153, 074112.	3.0	9
15	Molecular Mechanism of Flavin Photoprotection by Archaeal Dodecin: Photoinduced Electron Transfer and Mg²⁺-Promoted Proton Transfer. Journal of Physical Chemistry B, 2017, 121, 10457-10466.	2.6	7
16	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
17	Rethinking Uncaging: A New Antiaromatic Photocage Driven by a Gain of Resonance Energy. Chemistry - A European Journal, 2021, 27, 14121-14127.	3.3	7
18	A long-lived fluorenyl cation: efficiency booster for uncaging and photobase properties. Physical Chemistry Chemical Physics, 2022, 24, 5294-5300.	2.8	2

#	Article	IF	Citations
19	The rupture mechanism of rubredoxin is more complex than previously thought. Chemical Science, 2020, 11, 6036-6044.	7.4	1