Boyi Zhang

List of Publications by Year
in descending order

12	307	1163117 8	1281871 11
papers	citations	h-index	g-index

12	12	12	543
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Arbitrary-Order Derivatives of Quantum Chemical Methods via Automatic Differentiation. Journal of Physical Chemistry Letters, 2021, 12, 3232-3239.	4.6	16
2	A remarkable case of basis set dependence: the false convergence patterns of the methyl anion. Molecular Physics, 2019, 117, 1069-1077.	1.7	3
3	Janus: An Extensible Open-Source Software Package for Adaptive QM/MM Methods. Journal of Chemical Theory and Computation, 2019, 15, 4362-4373.	5.3	9
4	PES-Learn: An Open-Source Software Package for the Automated Generation of Machine Learning Models of Molecular Potential Energy Surfaces. Journal of Chemical Theory and Computation, 2019, 15, 4386-4398.	5.3	51
5	A Multireference Ab Initio Study of the Diradical Isomers of Pyrazine. Journal of Physical Chemistry A, 2019, 123, 2049-2057.	2.5	9
6	A comparison between hydrogen and halogen bonding: the hypohalous acidâ€“water dimers, HOXâ‹¯H₂O (X = F, Cl, Br). Physical Chemistry Chemical Physics, 2019, 21, 6160-6170.	2.8	28
7	Relatives of cyanomethylene: replacement of the divalent carbon by B^{â”}, N⁺, Al^{â”}, Si, P⁺, Ga^{â”}, Ge, and As⁺. Physical Chemistry Chemical Physics, 2019, 21, 26438-26452.	2.8	3
8	Spinâ€“Orbit Coupling via Four-Component Multireference Methods: Benchmarking on p-Block Elements and Tentative Recommendations. Journal of Chemical Theory and Computation, 2018, 14, 1235-1246.	5.3	15
9	An Extended Multireference Study of the Singlet and Triplet States of the 9,10-didehydroanthracene Diradical. Journal of Physical Chemistry A, 2018, 122, 3688-3696.	2.5	4
10	P<scp>si</scp>4N<scp>um</scp>P<scp>y</scp>: An Interactive Quantum Chemistry Programming Environment for Reference Implementations and Rapid Development. Journal of Chemical Theory and Computation, 2018, 14, 3504-3511.	5.3	106
11	Nanoaggregates of Diverse Asphaltenes by Mass Spectrometry and Molecular Dynamics. Energy & Fuels, 2017, 31, 9140-9151.	5.1	63
12	The isomerisation of H2XY to HXYH (X, Y = O, S, and Se)*. Molecular Physics, 0, , .	1.7	0