Chad E Hoyer

List of Publications by Year
in descending order

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20 papers	2,735 citations	566801 15 h-index	752256 20 g-index
24 all docs	24 docs citations	24 times ranked	3271 citing authors

#	Article	IF	Citations
1	Phaseâ€Controlled Synthesis and Quasiâ€Static Dielectric Resonances in Silver Iron Sulfide (AgFeS) Tj ETQq1 1 0.784314 rgBT /Overlock	3.2	2
2	Iron-Content-Dependent, Quasi-Static Dielectric Resonances and Oxidative Transitions in Bornite and Chalcopyrite Copper Iron Sulfide Nanocrystals. Chemistry of Materials, 2021, 33, 1821-1831.	3.2	17
3	The Chronus Quantum software package. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1436.	6.2	66
4	Relativistic two-component projection-based quantum embedding for open-shell systems. Journal of Chemical Physics, 2020, 153, 094113.	1.2	10
5	Embedding non-collinear two-component electronic structure in a collinear quantum environment. Journal of Chemical Physics, 2019, 150, 174114.	1.2	9
6	OpenMolcas: From Source Code to Insight. Journal of Chemical Theory and Computation, 2019, 15, 5925-5964.	2.3	661
7	Analytic Gradients for Complete Active Space Pair-Density Functional Theory. Journal of Chemical Theory and Computation, 2018, 14, 126-138.	2.3	40
8	State-interaction pair-density functional theory. Journal of Chemical Physics, 2018, 149, 024106.	1.2	27
9	Multiconfiguration Pair-Density Functional Theory: A New Way To Treat Strongly Correlated Systems. Accounts of Chemical Research, 2017, 50, 66-73.	7.6	232
10	The DQ and DQÎ¦ electronic structure diabatization methods: Validation for general applications. Journal of Chemical Physics, 2016, 144, 194101.	1.2	42
11	Comment on â€œFe2: As simple as a Herculean labour. Neutral (Fe2), cationic (Fe2+), and anionic (Fe2â^’) speciesâ€•[J. Chem. Phys. 142, 244304 (2015)]. Journal of Chemical Physics, 2016, 144, 027101.	1.2	2
12	<scp>Molcas</scp> 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. Journal of Computational Chemistry, 2016, 37, 506-541.	1.5	1,317
13	Multiconfiguration Pair-Density Functional Theory Is as Accurate as CASPT2 for Electronic Excitation. Journal of Physical Chemistry Letters, 2016, 7, 586-591.	2.1	75
14	Multiconfiguration Pair-Density Functional Theory Outperforms Kohnâ€“Sham Density Functional Theory and Multireference Perturbation Theory for Ground-State and Excited-State Charge Transfer. Journal of Chemical Theory and Computation, 2015, 11, 3643-3649.	2.3	40
15	Multiconfiguration Pair-Density Functional Theory Spectral Calculations Are Stable to Adding Diffuse Basis Functions. Journal of Physical Chemistry Letters, 2015, 6, 4184-4188.	2.1	22
16	Nonintuitive Diabatic Potential Energy Surfaces for Thioanisole. Journal of Physical Chemistry Letters, 2015, 6, 3352-3359.	2.1	17
17	Controversial electronic structures and energies of Fe2, ${m Fe}_2^ +$ Fe 2+, and ${m Fe}_2^ -$ Fe 2â^’ resolved by RASPT2 calculations. Journal of Chemical Physics, 2014, 141, 204309.	1.2	22
18	Diabatization based on the dipole and quadrupole: The DQ method. Journal of Chemical Physics, 2014, 141, 114104.	1.2	58

#	Article	IF	Citations
19	A Two-Coordinate Manganese(0) Complex with an Unsupported Mnâ€“Mg Bond: Allowing Access to Low Coordinate Homo- and Heterobimetallic Compounds. Journal of the American Chemical Society, 2014, 136, 5283-5286.	6.6	70
20	A Primer in Monte Carlo Integration Using Mathcad. Journal of Chemical Education, 2013, 90, 1186-1190.	1.1	2