

Chad E Hoyer

List of Publications by Year in descending order

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Version: 2024-02-01

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	<sc>Molcas</sc> 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. <i>Journal of Computational Chemistry</i> , 2016, 37, 506-541.	1.5	1,317
2	OpenMolcas: From Source Code to Insight. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 5925-5964.	2.3	661
3	Multiconfiguration Pair-Density Functional Theory: A New Way To Treat Strongly Correlated Systems. <i>Accounts of Chemical Research</i> , 2017, 50, 66-73.	7.6	232
4	Multiconfiguration Pair-Density Functional Theory Is as Accurate as CASPT2 for Electronic Excitation. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 586-591.	2.1	75
5	A Two-Coordinate Manganese(0) Complex with an Unsupported Mn-Mg Bond: Allowing Access to Low Coordinate Homo- and Heterobimetallic Compounds. <i>Journal of the American Chemical Society</i> , 2014, 136, 5283-5286.	6.6	70
6	The Chronus Quantum software package. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2020, 10, e1436.	6.2	66
7	Diabatization based on the dipole and quadrupole: The DQ method. <i>Journal of Chemical Physics</i> , 2014, 141, 114104.	1.2	58
8	The DQ and DQ [†] electronic structure diabatization methods: Validation for general applications. <i>Journal of Chemical Physics</i> , 2016, 144, 194101.	1.2	42
9	Multiconfiguration Pair-Density Functional Theory Outperforms Kohn-Sham Density Functional Theory and Multireference Perturbation Theory for Ground-State and Excited-State Charge Transfer. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 3643-3649.	2.3	40
10	Analytic Gradients for Complete Active Space Pair-Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 126-138.	2.3	40
11	State-interaction pair-density functional theory. <i>Journal of Chemical Physics</i> , 2018, 149, 024106.	1.2	27
12	Controversial electronic structures and energies of Fe ₂ , $\{m Fe\}_2^+ + Fe_2^+$, and $\{m Fe\}_2^- - Fe_2^-$ resolved by RASPT2 calculations. <i>Journal of Chemical Physics</i> , 2014, 141, 204309.	1.2	22
13	Multiconfiguration Pair-Density Functional Theory Spectral Calculations Are Stable to Adding Diffuse Basis Functions. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 4184-4188.	2.1	22
14	Nonintuitive Diabatic Potential Energy Surfaces for Thioanisole. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 3352-3359.	2.1	17
15	Iron-Content-Dependent, Quasi-Static Dielectric Resonances and Oxidative Transitions in Bornite and Chalcopyrite Copper Iron Sulfide Nanocrystals. <i>Chemistry of Materials</i> , 2021, 33, 1821-1831.	3.2	17
16	Relativistic two-component projection-based quantum embedding for open-shell systems. <i>Journal of Chemical Physics</i> , 2020, 153, 094113.	1.2	10
17	Embedding non-collinear two-component electronic structure in a collinear quantum environment. <i>Journal of Chemical Physics</i> , 2019, 150, 174114.	1.2	9
18	A Primer in Monte Carlo Integration Using Mathcad. <i>Journal of Chemical Education</i> , 2013, 90, 1186-1190.	1.1	2

#	ARTICLE	IF	CITATIONS
19	Comment on "Fe ₂ : As simple as a Herculean labour. Neutral (Fe ₂), cationic (Fe ₂ ⁺), and anionic (Fe ₂ ⁻) species". J. Chem. Phys. 142 , 244304 (2015). Journal of Chemical Physics, 2016, 144, 027101.	1.2	2
20	Phase-Controlled Synthesis and Quasi-Static Dielectric Resonances in Silver Iron Sulfide (AgFeS)	3.2	2