

Caroline M Krauter

List of Publications by Year in descending order

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Version: 2024-02-01

17
papers

4,422
citations

623188

14
h-index

887659

17
g-index

18
all docs

18
docs citations

18
times ranked

5750
citing authors

#	ARTICLE	IF	CITATIONS
1	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. <i>Molecular Physics</i> , 2015, 113, 184-215.	0.8	2,561
2	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. <i>Journal of Chemical Physics</i> , 2021, 155, 084801.	1.2	518
3	Heterometallic antenna-reactor complexes for photocatalysis. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016, 113, 8916-8920.	3.3	381
4	Aluminum Nanocrystals as a Plasmonic Photocatalyst for Hydrogen Dissociation. <i>Nano Letters</i> , 2016, 16, 1478-1484.	4.5	294
5	Investigating excited electronic states using the algebraic diagrammatic construction (ADC) approach of the polarisation propagator. <i>Molecular Physics</i> , 2014, 112, 774-784.	0.8	169
6	How To Identify Plasmons from the Optical Response of Nanostructures. <i>ACS Nano</i> , 2017, 11, 7321-7335.	7.3	72
7	Stereoselective Synthesis of 2,6-Disubstituted Piperidines Using the Iridium-Catalyzed Allylic Cyclization as Configurational Switch: Asymmetric Total Synthesis of (+)- ϵ -241 and Related Piperidine Alkaloids. <i>Chemistry - A European Journal</i> , 2009, 15, 2050-2054.	1.7	62
8	A Configurational Switch Based on Iridium-Catalyzed Allylic Cyclization: Application in Asymmetric Total Syntheses of Prosopis, Dendrobate, and Spruce Alkaloids. <i>Chemistry - A European Journal</i> , 2009, 15, 10514-10532.	1.7	58
9	Application of the scaled-opposite-spin approximation to algebraic diagrammatic construction schemes of second order. <i>Journal of Chemical Physics</i> , 2013, 138, 044107.	1.2	53
10	Ultrafast branching in the excited state of coumarin and umbelliferone. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 17846.	1.3	48
11	Understanding the apparent fractional charge of protons in the aqueous electrochemical double layer. <i>Nature Communications</i> , 2018, 9, 3202.	5.8	47
12	Ab Initio Kinetics of Hydrogen Abstraction from Methyl Acetate by Hydrogen, Methyl, Oxygen, Hydroxyl, and Hydroperoxy Radicals. <i>Journal of Physical Chemistry A</i> , 2015, 119, 6377-6390.	1.1	43
13	Identification of Plasmons in Molecules with Scaled Ab Initio Approaches. <i>Journal of Physical Chemistry C</i> , 2015, 119, 24564-24573.	1.5	34
14	Plasmons in molecules: Microscopic characterization based on orbital transitions and momentum conservation. <i>Journal of Chemical Physics</i> , 2014, 141, 104101.	1.2	26
15	Density Fitting and Cholesky Decomposition of the Two-Electron Integrals in Local Multireference Configuration Interaction Theory. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 5242-5251.	2.3	14
16	Algebraic diagrammatic construction for the polarization propagator with spin-orbit coupling. <i>Chemical Physics</i> , 2017, 482, 286-293.	0.9	9
17	Corrigendum to: Plasmon-Driven Dissociation of H ₂ on Gold Nanoclusters. <i>Zeitschrift Fur Physikalische Chemie</i> , 2016, 230, 131-132.	1.4	8