Caroline M Krauter

List of Publications by Year
in descending order

17	4,422	623188 14	887659 17
papers	citations	h-index	g-index

18	18	18	5750
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.	1.2	518
2	Understanding the apparent fractional charge of protons in the aqueous electrochemical double layer. Nature Communications, 2018, 9, 3202.	5.8	47
3	How To Identify Plasmons from the Optical Response of Nanostructures. ACS Nano, 2017, 11, 7321-7335.	7.3	72
4	Algebraic diagrammatic construction for the polarization propagator with spin-orbit coupling. Chemical Physics, 2017, 482, 286-293.	0.9	9
5	Heterometallic antennaâ^'reactor complexes for photocatalysis. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 8916-8920.	3.3	381
6	Aluminum Nanocrystals as a Plasmonic Photocatalyst for Hydrogen Dissociation. Nano Letters, 2016, 16, 1478-1484.	4.5	294
7	Corrigendum to: Plasmon-Driven Dissociation of H₂ on Gold Nanoclusters. Zeitschrift Fur Physikalische Chemie, 2016, 230, 131-132.	1.4	8
8	Ab Initio Kinetics of Hydrogen Abstraction from Methyl Acetate by Hydrogen, Methyl, Oxygen, Hydroxyl, and Hydroperoxy Radicals. Journal of Physical Chemistry A, 2015, 119, 6377-6390.	1.1	43
9	Identification of Plasmons in Molecules with Scaled Ab Initio Approaches. Journal of Physical Chemistry C, 2015, 119, 24564-24573.	1.5	34
10	Density Fitting and Cholesky Decomposition of the Two-Electron Integrals in Local Multireference Configuration Interaction Theory. Journal of Chemical Theory and Computation, 2015, 11, 5242-5251.	2.3	14
11	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	0.8	2,561
12	Plasmons in molecules: Microscopic characterization based on orbital transitions and momentum conservation. Journal of Chemical Physics, 2014, 141, 104101.	1.2	26
13	Investigating excited electronic states using the algebraic diagrammatic construction (ADC) approach of the polarisation propagator. Molecular Physics, 2014, 112, 774-784.	0.8	169
14	Ultrafast branching in the excited state of coumarin and umbelliferone. Physical Chemistry Chemical Physics, 2013, 15, 17846.	1.3	48
15	Application of the scaled-opposite-spin approximation to algebraic diagrammatic construction schemes of second order. Journal of Chemical Physics, 2013, 138, 044107.	1.2	53
16	Stereoselective Synthesis of 2,6â€Disubstituted Piperidines Using the Iridiumâ€Catalyzed Allylic Cyclization as Configurational Switch: Asymmetric Total Synthesis of (+)â€241â€‰D and Related Piperidine Alkaloids. Chemistry - A European Journal, 2009, 15, 2050-2054.	1.7	62
17	A Configurational Switch Based on Iridiumâ€Catalyzed Allylic Cyclization: Application in Asymmetric Total Syntheses of Prosopis, Dendrobate, and Spruce Alkaloids. Chemistry - A European Journal, 2009, 15, 10514-10532.	1.7	58