Reed Nieman

List of Publications by Year
in descending order

22 papers	365 citations	1040056 9 h-index	794594 19 g-index
22 all docs	22 docs citations	22 times ranked	623 citing authors

#	Article	IF	Citations
1	Ab Initio Modeling of Excitonic and Charge-Transfer States in Organic Semiconductors: The PTB1/PCBM Low Band Gap System. Journal of the American Chemical Society, 2013, 135, 18252-18255.	13.7	59
2	Comparison of LC-TDDFT and ADC(2) Methods in Computations of Bright and Charge Transfer States in Stacked Oligothiophenes. Journal of Chemical Theory and Computation, 2014, 10, 3280-3289.	5.3	54
3	Intermolecular interactions and charge transfer transitions in aromatic hydrocarbonâ€“tetracyanoethylene complexes. Physical Chemistry Chemical Physics, 2014, 16, 20586-20597.	2.8	43
4	The generality of the GUGA MRCI approach in COLUMBUS for treating complex quantum chemistry. Journal of Chemical Physics, 2020, 152, 134110.	3.0	42
5	Diradical Organic Oneâ€Dimensional Polymers Synthesized on a Metallic Surface. Angewandte Chemie - International Edition, 2020, 59, 17594-17599.	13.8	33
6	Interplay of Biradicaloid Character and Singlet/Triplet Energy Splitting for cis-/trans-Diindenoacenes and Related Benzothiophene-Capped Oligomers as Revealed by Extended Multireference Calculations. Journal of Organic Chemistry, 2020, 85, 3664-3675.	3.2	16
7	Diradical Organic Oneâ€Dimensional Polymers Synthesized on a Metallic Surface. Angewandte Chemie, 2020, 132, 17747-17752.	2.0	14
8	Characterization of glycan isomers using magnetic carbon nanoparticles as a MALDI co-matrix. RSC Advances, 2019, 9, 20137-20148.	3.6	13
9	Exploring reactivity and product formation in N(4S) collisions with pristine and defected graphene with direct dynamics simulations. Journal of Chemical Physics, 2020, 153, 184702.	3.0	13
10	Direct Dynamics Simulations of Hyperthermal O(3P) Collisions with Pristine, Defected, Oxygenated, and Nitridated Graphene Surfaces. Journal of Physical Chemistry C, 2021, 125, 9795-9808.	3.1	10
11	Exploration of Graphene Defect Reactivity toward a Hydrogen Radical Utilizing a Preactivated Circumcoronene Model. Journal of Physical Chemistry A, 2021, 125, 1152-1165.	2.5	10
12	Structure and electronic states of a graphene double vacancy with an embedded Si dopant. Journal of Chemical Physics, 2017, 147, 194702.	3.0	9
13	Single and double carbon vacancies in pyrene as first models for graphene defects: A survey of the chemical reactivity toward hydrogen. Chemical Physics, 2017, 482, 346-354.	1.9	9
14	A Multireference Ab Initio Study of the Diradical Isomers of Pyrazine. Journal of Physical Chemistry A, 2019, 123, 2049-2057.	2.5	9
15	Photoacidity of the 7â€Hydroxyflavylium Cation. Photochemistry and Photobiology, 2019, 95, 1339-1344.	2.5	6
16	The crucial role of a spacer material on the efficiency of charge transfer processes in organic donorâ€“acceptor junction solar cells. Nanoscale, 2018, 10, 451-459.	5.6	5
17	Benchmark ab initio calculations on intermolecular structures and the exciton character of poly(p-phenylenevinylene) dimers. Journal of Chemical Physics, 2020, 152, 044306.	3.0	5
18	Insights into adsorption, diffusion, and reactions of atomic nitrogen on a highly oriented pyrolytic graphite surface. Journal of Chemical Physics, 2021, 154, 074708.	3.0	5

#	Article	IF	Citations
19	A general new method for calculating the molecular nonpolar surface for analysis of LC-MS data. International Journal of Mass Spectrometry, 2021, 461, 116495.	1.5	3
20	Spin-density calculation via the graphical unitary group approach. Molecular Physics, 2023, 121, .	1.7	3
21	Reaction mechanism for fluorination reactions with hydroxylated alumina sites: Pathways promoting aluminum combustion. Journal of Chemical Physics, 2021, 154, 104308.	3.0	2
22	Quantum chemical investigation of the ground- and excited-state acidities of a dihydroxyfuranoflavylium cation. Theoretical Chemistry Accounts, 2021, 140, 1.	1.4	2