

# Reed Nieman

## List of Publications by Year in descending order

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Version: 2024-02-01

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	Spin-density calculation via the graphical unitary group approach. <i>Molecular Physics</i> , 2023, 121, .	1.7	3
2	Insights into adsorption, diffusion, and reactions of atomic nitrogen on a highly oriented pyrolytic graphite surface. <i>Journal of Chemical Physics</i> , 2021, 154, 074708.	3.0	5
3	A general new method for calculating the molecular nonpolar surface for analysis of LC-MS data. <i>International Journal of Mass Spectrometry</i> , 2021, 461, 116495.	1.5	3
4	Reaction mechanism for fluorination reactions with hydroxylated alumina sites: Pathways promoting aluminum combustion. <i>Journal of Chemical Physics</i> , 2021, 154, 104308.	3.0	2
5	Direct Dynamics Simulations of Hyperthermal O(3P) Collisions with Pristine, Defected, Oxygenated, and Nitridated Graphene Surfaces. <i>Journal of Physical Chemistry C</i> , 2021, 125, 9795-9808.	3.1	10
6	Quantum chemical investigation of the ground- and excited-state acidities of a dihydroxyfuranoflavylium cation. <i>Theoretical Chemistry Accounts</i> , 2021, 140, 1.	1.4	2
7	Exploration of Graphene Defect Reactivity toward a Hydrogen Radical Utilizing a Preactivated Circumcoronene Model. <i>Journal of Physical Chemistry A</i> , 2021, 125, 1152-1165.	2.5	10
8	Exploring reactivity and product formation in N(4S) collisions with pristine and defected graphene with direct dynamics simulations. <i>Journal of Chemical Physics</i> , 2020, 153, 184702.	3.0	13
9	Diradical Organic One-Dimensional Polymers Synthesized on a Metallic Surface. <i>Angewandte Chemie</i> , 2020, 132, 17747-17752.	2.0	14
10	Diradical Organic One-Dimensional Polymers Synthesized on a Metallic Surface. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 17594-17599.	13.8	33
11	Interplay of Biradicaloid Character and Singlet/Triplet Energy Splitting for <i>cis</i> -/ <i>trans</i> -Diindenoacenes and Related Benzothiophene-Capped Oligomers as Revealed by Extended Multireference Calculations. <i>Journal of Organic Chemistry</i> , 2020, 85, 3664-3675.	3.2	16
12	Benchmark ab initio calculations on intermolecular structures and the exciton character of poly( <i>p</i> -phenylenevinylene) dimers. <i>Journal of Chemical Physics</i> , 2020, 152, 044306.	3.0	5
13	The generality of the GUGA MRCI approach in COLUMBUS for treating complex quantum chemistry. <i>Journal of Chemical Physics</i> , 2020, 152, 134110.	3.0	42
14	Characterization of glycan isomers using magnetic carbon nanoparticles as a MALDI co-matrix. <i>RSC Advances</i> , 2019, 9, 20137-20148.	3.6	13
15	Photoacidity of the 7-Hydroxyflavylium Cation. <i>Photochemistry and Photobiology</i> , 2019, 95, 1339-1344.	2.5	6
16	A Multireference Ab Initio Study of the Diradical Isomers of Pyrazine. <i>Journal of Physical Chemistry A</i> , 2019, 123, 2049-2057.	2.5	9
17	The crucial role of a spacer material on the efficiency of charge transfer processes in organic donor-acceptor junction solar cells. <i>Nanoscale</i> , 2018, 10, 451-459.	5.6	5
18	Structure and electronic states of a graphene double vacancy with an embedded Si dopant. <i>Journal of Chemical Physics</i> , 2017, 147, 194702.	3.0	9

#	ARTICLE	IF	CITATIONS
19	Single and double carbon vacancies in pyrene as first models for graphene defects: A survey of the chemical reactivity toward hydrogen. <i>Chemical Physics</i> , 2017, 482, 346-354.	1.9	9
20	Intermolecular interactions and charge transfer transitions in aromatic hydrocarbon-tetracyanoethylene complexes. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 20586-20597.	2.8	43
21	Comparison of LC-TDDFT and ADC(2) Methods in Computations of Bright and Charge Transfer States in Stacked Oligothiophenes. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 3280-3289.	5.3	54
22	<i>Ab Initio</i> Modeling of Excitonic and Charge-Transfer States in Organic Semiconductors: The PTB1/PCBM Low Band Gap System. <i>Journal of the American Chemical Society</i> , 2013, 135, 18252-18255.	13.7	59