

# Alec F White

## List of Publications by Year in descending order

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Version: 2024-02-01

19  
papers

3,896  
citations

566801

15  
h-index

752256

20  
g-index

25  
all docs

25  
docs citations

25  
times ranked

4395  
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	Recent developments in the P<sc>y</sc>SCF program package. <i>Journal of Chemical Physics</i> , 2020, 153, 024109.	1.2	388
4	Computation of high-harmonic generation spectra of the hydrogen molecule using time-dependent configuration-interaction. <i>Molecular Physics</i> , 2016, 114, 947-956.	0.8	47
5	A Time-Dependent Formulation of Coupled-Cluster Theory for Many-Fermion Systems at Finite Temperature. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 5690-5700.	2.3	47
6	Complex basis functions revisited: Implementation with applications to carbon tetrafluoride and aromatic N-containing heterocycles within the static-exchange approximation. <i>Journal of Chemical Physics</i> , 2015, 142, 054103.	1.2	46
7	Non-orthogonal configuration interaction with single substitutions for the calculation of core-excited states. <i>Journal of Chemical Physics</i> , 2018, 149, 044116.	1.2	44
8	Non-Orthogonal Configuration Interaction with Single Substitutions for Core-Excited States: An Extension to Doublet Radicals. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 2966-2973.	2.3	39
9	Second order MÅller-Plesset and coupled cluster singles and doubles methods with complex basis functions for resonances in electron-molecule scattering. <i>Journal of Chemical Physics</i> , 2017, 146, 234107.	1.2	36
10	Restricted and unrestricted non-Hermitian Hartree-Fock: Theory, practical considerations, and applications to metastable molecular anions. <i>Journal of Chemical Physics</i> , 2015, 143, 074103.	1.2	31
11	Electronic structure of bulk manganese oxide and nickel oxide from coupled cluster theory. <i>Physical Review B</i> , 2020, 101, .	1.1	27
12	A coupled cluster framework for electrons and phonons. <i>Journal of Chemical Physics</i> , 2020, 153, 224112.	1.2	17
13	Stabilizing potentials in bound state analytic continuation methods for electronic resonances in polyatomic molecules. <i>Journal of Chemical Physics</i> , 2017, 146, 044112.	1.2	16
14	Finite-temperature coupled cluster: Efficient implementation and application to prototypical systems. <i>Journal of Chemical Physics</i> , 2020, 152, 224104.	1.2	16
15	Generalized single excitation configuration interaction: an investigation into the impact of the inclusion of non-orthogonality on the calculation of core-excited states. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 8182-8192.	1.3	16
16	Time-Dependent Coupled Cluster Theory on the Keldysh Contour for Nonequilibrium Systems. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 6137-6153.	2.3	15
17	Probing Ionic Complexes of Ethylene and Acetylene with Vacuum-Ultraviolet Radiation. <i>Journal of Physical Chemistry A</i> , 2016, 120, 5053-5064.	1.1	11
18	Simulating the absorption spectra of helium clusters (N=70, 150, 231, 300) using a charge transfer correction to superposition of fragment single excitations. <i>Journal of Chemical Physics</i> , 2017, 146, 044111.	1.2	11

#	ARTICLE	IF	CITATIONS
19	Conservation laws in coupled cluster dynamics at finite temperature. Journal of Chemical Physics, 2021, 155, 044103.	1.2	7