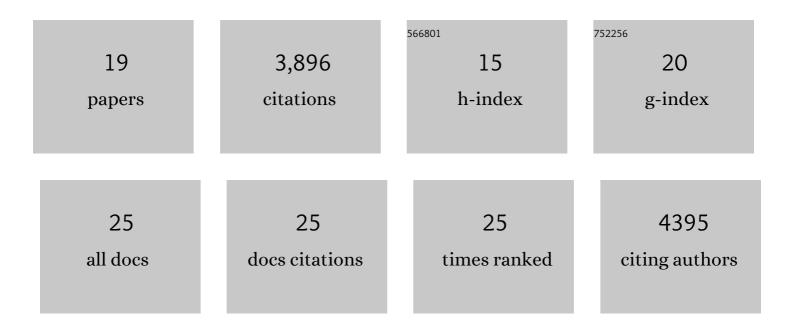
## Alec F White

List of Publications by Year in descending order

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ALEC F MULTE

#	Article	IF	CITATIONS
1	Conservation laws in coupled cluster dynamics at finite temperature. Journal of Chemical Physics, 2021, 155, 044103.	1.2	7
2	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
3	Recent developments in the P <scp>y</scp> SCF program package. Journal of Chemical Physics, 2020, 153, 024109.	1.2	388
4	Finite-temperature coupled cluster: Efficient implementation and application to prototypical systems. Journal of Chemical Physics, 2020, 152, 224104.	1.2	16
5	Electronic structure of bulk manganese oxide and nickel oxide from coupled cluster theory. Physical Review B, 2020, 101, .	1.1	27
6	Generalized single excitation configuration interaction: an investigation into the impact of the inclusion of non-orthogonality on the calculation of core-excited states. Physical Chemistry Chemical Physics, 2020, 22, 8182-8192.	1.3	16
7	A coupled cluster framework for electrons and phonons. Journal of Chemical Physics, 2020, 153, 224112.	1.2	17
8	Time-Dependent Coupled Cluster Theory on the Keldysh Contour for Nonequilibrium Systems. Journal of Chemical Theory and Computation, 2019, 15, 6137-6153.	2.3	15
9	Non-Orthogonal Configuration Interaction with Single Substitutions for Core-Excited States: An Extension to Doublet Radicals. Journal of Chemical Theory and Computation, 2019, 15, 2966-2973.	2.3	39
10	A Time-Dependent Formulation of Coupled-Cluster Theory for Many-Fermion Systems at Finite Temperature. Journal of Chemical Theory and Computation, 2018, 14, 5690-5700.	2.3	47
11	Non-orthogonal configuration interaction with single substitutions for the calculation of core-excited states. Journal of Chemical Physics, 2018, 149, 044116.	1.2	44
12	Simulating the absorption spectra of helium clusters (N = 70, 150, 231, 300) using a charge transfer correction to superposition of fragment single excitations. Journal of Chemical Physics, 2017, 146, 044111.	1.2	11
13	Stabilizing potentials in bound state analytic continuation methods for electronic resonances in polyatomic molecules. Journal of Chemical Physics, 2017, 146, 044112.	1.2	16
14	Second order MÃ,ller-Plesset and coupled cluster singles and doubles methods with complex basis functions for resonances in electron-molecule scattering. Journal of Chemical Physics, 2017, 146, 234107.	1.2	36
15	Probing Ionic Complexes of Ethylene and Acetylene with Vacuum-Ultraviolet Radiation. Journal of Physical Chemistry A, 2016, 120, 5053-5064.	1.1	11
16	Computation of high-harmonic generation spectra of the hydrogen molecule using time-dependent configuration-interaction. Molecular Physics, 2016, 114, 947-956.	0.8	47
17	Restricted and unrestricted non-Hermitian Hartree-Fock: Theory, practical considerations, and applications to metastable molecular anions. Journal of Chemical Physics, 2015, 143, 074103.	1.2	31
18	Complex basis functions revisited: Implementation with applications to carbon tetrafluoride and aromatic N-containing heterocycles within the static-exchange approximation. Journal of Chemical Physics, 2015, 142, 054103.	1.2	46

#	Article	IF	CITATIONS
19	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	0.8	2,561