# Alec F White

List of Publications by Year
in descending order



| | | | |
|---|---|---|---|
| 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 | 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 (Nâ€‰=â€‰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 |