David B Williams-Young

List of Publications by Year
in descending order

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26 papers	572 citations	623734 14 h-index	610901 24 g-index
26 all docs	26 docs citations	26 times ranked	487 citing authors

#	Article	IF	Citations
1	The Chronus Quantum software package. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1436.	14.6	66
2	An efficient implementation of two-component relativistic density functional theory with torque-free auxiliary variables. European Physical Journal B, 2018, 91, 1.	1.5	54
3	Direct ab Initio (Meta-)Surface-Hopping Dynamics. Journal of Chemical Theory and Computation, 2016, 12, 935-945.	5.3	40
4	Relativistic Real-Time Time-Dependent Equation-of-Motion Coupled-Cluster. Journal of Chemical Theory and Computation, 2019, 15, 6617-6624.	5.3	40
5	From NWChem to NWChemEx: Evolving with the Computational Chemistry Landscape. Chemical Reviews, 2021, 121, 4962-4998.	47.7	39
6	Ab Initio Transient Vibrational Spectral Analysis. Journal of Physical Chemistry Letters, 2016, 7, 4501-4508.	4.6	37
7	Generalized Hartreeâ€“Fock with Nonperturbative Treatment of Strong Magnetic Fields: Application to Molecular Spin Phase Transitions. Journal of Chemical Theory and Computation, 2019, 15, 348-356.	5.3	33
8	An ab Initio Linear Response Method for Computing Magnetic Circular Dichroism Spectra with Nonperturbative Treatment of Magnetic Field. Journal of Chemical Theory and Computation, 2019, 15, 3162-3169.	5.3	27
9	Accurate Assignments of Excited-State Resonance Raman Spectra: A Benchmark Study Combining Experiment and Theory. Journal of Physical Chemistry A, 2017, 121, 7937-7946.	2.5	26
10	Effective Inclusion of Mechanical and Electrical Anharmonicity in Excited Electronic States: VPT2-TDDFT Route. Journal of Chemical Theory and Computation, 2017, 13, 2789-2803.	5.3	23
11	Simulating Magnetic Circular Dichroism Spectra with Real-Time Time-Dependent Density Functional Theory in Gauge Including Atomic Orbitals. Journal of Chemical Theory and Computation, 2019, 15, 6824-6831.	5.3	19
12	Accelerating Real-Time Time-Dependent Density Functional Theory with a Nonrecursive Chebyshev Expansion of the Quantum Propagator. Journal of Chemical Theory and Computation, 2016, 12, 5333-5338.	5.3	18
13	Approximate Greenâ€™s Function Coupled Cluster Method Employing Effective Dimension Reduction. Journal of Chemical Theory and Computation, 2019, 15, 3185-3196.	5.3	17
14	Ab Initio Excited-State Transient Raman Analysis. Journal of Physical Chemistry A, 2017, 121, 3958-3965.	2.5	16
15	A Well-Tempered Hybrid Method for Solving Challenging Time-Dependent Density Functional Theory (TDDFT) Systems. Journal of Chemical Theory and Computation, 2018, 14, 2034-2041.	5.3	15
16	Model Order Reduction Algorithm for Estimating the Absorption Spectrum. Journal of Chemical Theory and Computation, 2017, 13, 4950-4961.	5.3	14
17	Efficient Implementation of Variation after Projection Generalized Hartreeâ€“Fock. Journal of Chemical Theory and Computation, 2018, 14, 588-596.	5.3	14
18	Relativistic Two-Component Particleâ€“Particle Tammâ€“Dancoff Approximation. Journal of Chemical Theory and Computation, 2016, 12, 5379-5384.	5.3	13

#	Article	IF	Citations
19	Modeling Magnetoâ€Photoabsorption Using Timeâ€Dependent Complex Generalized Hartreeâ€Fock. ChemPhotoChem, 2019, 3, 739-746.	3.0	11
20	On the Efficient Evaluation of the Exchange Correlation Potential on Graphics Processing Unit Clusters. Frontiers in Chemistry, 2020, 8, 581058.	3.6	11
21	The Effect of Geometry, Spin, and Orbital Optimization in Achieving Accurate, Correlated Results for Ironâ€“Sulfur Cubanes. Journal of Chemical Theory and Computation, 2022, 18, 687-702.	5.3	10
22	Embedding non-collinear two-component electronic structure in a collinear quantum environment. Journal of Chemical Physics, 2019, 150, 174114.	3.0	9
23	Achieving performance portability in Gaussian basis set density functional theory on accelerator based architectures in NWChemEx. Parallel Computing, 2021, 108, 102829.	2.1	7
24	Solving Coupled Cluster Equations by the Newton Krylov Method. Frontiers in Chemistry, 2020, 8, 590184.	3.6	6
25	A Shift Selection Strategy for Parallel Shift-invert Spectrum Slicing in Symmetric Self-consistent Eigenvalue Computation. ACM Transactions on Mathematical Software, 2020, 46, 1-31.	2.9	4
26	Parallel Shift-Invert Spectrum Slicing on Distributed Architectures with GPU Accelerators. , 2020, , .		3