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 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
2	From NWChem to NWChemEx: Evolving with the Computational Chemistry Landscape. Chemical Reviews, 2021, 121, 4962-4998.	47.7	39
3	Achieving performance portability in Gaussian basis set density functional theory on accelerator based architectures in NWChemEx. Parallel Computing, 2021, 108, 102829.	2.1	7
4	The Chronus Quantum software package. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1436.	14.6	66
5	Parallel Shift-Invert Spectrum Slicing on Distributed Architectures with GPU Accelerators. , 2020, , .		3
6	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
7	On the Efficient Evaluation of the Exchange Correlation Potential on Graphics Processing Unit Clusters. Frontiers in Chemistry, 2020, 8, 581058.	3.6	11
8	Solving Coupled Cluster Equations by the Newton Krylov Method. Frontiers in Chemistry, 2020, 8, 590184.	3.6	6
9	Embedding non-collinear two-component electronic structure in a collinear quantum environment. Journal of Chemical Physics, 2019, 150, 174114.	3.0	9
10	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
11	Relativistic Real-Time Time-Dependent Equation-of-Motion Coupled-Cluster. Journal of Chemical Theory and Computation, 2019, 15, 6617-6624.	5.3	40
12	Modeling Magnetoâ€Photoabsorption Using Timeâ€Dependent Complex Generalized Hartreeâ€Fock. ChemPhotoChem, 2019, 3, 739-746.	3.0	11
13	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
14	Approximate Greenâ€™s Function Coupled Cluster Method Employing Effective Dimension Reduction. Journal of Chemical Theory and Computation, 2019, 15, 3185-3196.	5.3	17
15	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
16	Efficient Implementation of Variation after Projection Generalized Hartreeâ€“Fock. Journal of Chemical Theory and Computation, 2018, 14, 588-596.	5.3	14
17	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
18	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

#	Article	IF	Citations
19	Ab Initio Excited-State Transient Raman Analysis. Journal of Physical Chemistry A, 2017, 121, 3958-3965.	2.5	16
20	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
21	Model Order Reduction Algorithm for Estimating the Absorption Spectrum. Journal of Chemical Theory and Computation, 2017, 13, 4950-4961.	5.3	14
22	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
23	Relativistic Two-Component Particleâ€“Particle Tammâ€“Dancoff Approximation. Journal of Chemical Theory and Computation, 2016, 12, 5379-5384.	5.3	13
24	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
25	Ab Initio Transient Vibrational Spectral Analysis. Journal of Physical Chemistry Letters, 2016, 7, 4501-4508.	4.6	37
26	Direct ab Initio (Meta-)Surface-Hopping Dynamics. Journal of Chemical Theory and Computation, 2016, 12, 935-945.	5.3	40