Dirk R Rehn

List of Publications by Year
in descending order

24 papers	3,633 citations	686830 13 h-index	610482 24 g-index
29 all docs	29 docs citations	29 times ranked	4173 citing authors

#	Article	IF	Citations
1	Quantum Monte Carlo formulation of the second order algebraic diagrammatic construction: Toward a massively parallel correlated excited state method. Journal of Chemical Physics, 2022, 156, 044105.	1.2	1
2	Exploring the accuracy and usefulness of semi-empirically scaled ADC schemes by blending second and third order terms. Journal of Chemical Physics, 2022, 156, 144101.	1.2	6
3	Electronic circular dichroism spectra using the algebraic diagrammatic construction schemes of the polarization propagator up to third order. Journal of Chemical Physics, 2021, 154, 064107.	1.2	12
4	Gator: A Python‑driven program for spectroscopy simulations using correlated wave functions. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1528.	6.2	16
5	Unitary coupled-cluster approach for the calculation of core-excited states and x-ray absorption spectra. Journal of Chemical Physics, 2021, 154, 154108.	1.2	4
6	*Ab Initio* Excited-State Electronic Circular Dichroism Spectra Exploiting the Third-Order Algebraic-Diagrammatic Construction Scheme for the Polarization Propagator. Journal of Physical Chemistry Letters, 2021, 12, 5132-5137.	2.1	8
7	Analytical gradients for core-excited states in the algebraic diagrammatic construction (ADC) framework. Journal of Chemical Physics, 2021, 155, 044106.	1.2	4
8	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
9	adcc: A versatile toolkit for rapid development of algebraic‑diagrammatic construction methods. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1462.	6.2	38
10	Complex excited state polarizabilities in the ADC/ISR framework. Journal of Chemical Physics, 2020, 153, 074112.	1.2	9
11	Third-Order Unitary Coupled Cluster (UCC3) for Excited Electronic States: Efficient Implementation and Benchmarking. Journal of Chemical Theory and Computation, 2020, 16, 3654-3663.	2.3	11
12	Hermitian second-order methods for excited electronic states: Unitary coupled cluster in comparison with algebraic‑diagrammatic construction schemes. Journal of Chemical Physics, 2020, 152, 094106.	1.2	12
13	Analytic nuclear gradients of the algebraic-diagrammatic construction scheme for the polarization propagator up to third order of perturbation theory. Journal of Chemical Physics, 2019, 150, 174110.	1.2	8
14	Similarities and differences of the Lagrange formalism and the intermediate state representation in the treatment of molecular properties. Journal of Chemical Physics, 2019, 150, 164125.	1.2	15
15	Nuclear dynamics in resonant inelastic X-ray scattering and X-ray absorption of methanol. Journal of Chemical Physics, 2019, 150, 234301.	1.2	26
16	Algebraic-diagrammatic construction scheme for the polarization propagator including ground-state coupled-cluster amplitudes. II. Static polarizabilities. Journal of Chemical Physics, 2019, 150, 174105.	1.2	13
17	Algebraic-diagrammatic construction scheme for the polarization propagator including ground-state coupled-cluster amplitudes. I. Excitation energies. Journal of Chemical Physics, 2019, 150, 174104.	1.2	11
18	Static polarizabilities and C6 dispersion coefficients using the algebraic-diagrammatic construction scheme for the complex polarization propagator. Journal of Chemical Physics, 2017, 146, .	1.2	30

#	Article	IF	Citations
19	Resonant Inelastic X-ray Scattering Amplitudes and Cross Sections in the Algebraic Diagrammatic Construction/Intermediate State Representation (ADC/ISR) Approach. Journal of Chemical Theory and Computation, 2017, 13, 5552-5559.	2.3	40
20	Accurate adiabatic singlet-triplet gaps in atoms and molecules employing the third-order spin-flip algebraic diagrammatic construction scheme for the polarization propagator. Journal of Chemical Physics, 2016, 145, 084102.	1.2	13
21	Benchmarking Post-Hartree–Fock Methods To Describe the Nonlinear Optical Properties of Polymethines: An Investigation of the Accuracy of Algebraic Diagrammatic Construction (ADC) Approaches. Journal of Chemical Theory and Computation, 2016, 12, 5465-5476.	2.3	13
22	Statistical analysis of electronic excitation processes: Spatial location, compactness, charge transfer, and electron-hole correlation. Journal of Computational Chemistry, 2015, 36, 1609-1620.	1.5	95
23	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	0.8	2,561
24	Investigating excited electronic states using the algebraic diagrammatic construction (ADC) approach of the polarisation propagator. Molecular Physics, 2014, 112, 774-784.	0.8	169