Dirk R Rehn

List of Publications by Year
in descending order

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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	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	0.8	2,561
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	Investigating excited electronic states using the algebraic diagrammatic construction (ADC) approach of the polarisation propagator. Molecular Physics, 2014, 112, 774-784.	0.8	169
4	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
5	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
6	adcc: A versatile toolkit for rapid development of algebraicâ€diagrammatic construction methods. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1462.	6.2	38
7	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
8	Nuclear dynamics in resonant inelastic X-ray scattering and X-ray absorption of methanol. Journal of Chemical Physics, 2019, 150, 234301.	1.2	26
9	Gator: A Pythonâ€driven program for spectroscopy simulations using correlated wave functions. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1528.	6.2	16
10	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
11	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
12	Benchmarking Post-Hartreeâ€“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
13	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
14	Hermitian second-order methods for excited electronic states: Unitary coupled cluster in comparison with algebraicâ€“diagrammatic construction schemes. Journal of Chemical Physics, 2020, 152, 094106.	1.2	12
15	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
16	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
17	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
18	Complex excited state polarizabilities in the ADC/ISR framework. Journal of Chemical Physics, 2020, 153, 074112.	1.2	9

#	Article	IF	Citations
19	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
20	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
21	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
22	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
23	Analytical gradients for core-excited states in the algebraic diagrammatic construction (ADC) framework. Journal of Chemical Physics, 2021, 155, 044106.	1.2	4
24	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