Rasmus Faber

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/1688546/publications.pdf

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20	451	623734	713466
papers	citations	14	21
		h-index	g-index

23	23	23	566
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Dalton Project: A Python platform for molecular- and electronic-structure simulations of complex systems. Journal of Chemical Physics, 2020, 152, 214115.	3.0	45
2	How to stay out of trouble in RIXS calculations within equation-of-motion coupled-cluster damped response theory? Safe hitchhiking in the excitation manifold by means of coreâ€“valence separation. Physical Chemistry Chemical Physics, 2020, 22, 2629-2641.	2.8	42
3	Importance of Triples Contributions to NMR Spinâ€“Spin Coupling Constants Computed at the CC3 and CCSDT Levels. Journal of Chemical Theory and Computation, 2017, 13, 696-709.	5.3	41
4	Resonant Inelastic X-ray Scattering and Nonesonant X-ray Emission Spectra from Coupled-Cluster (Damped) Response Theory. Journal of Chemical Theory and Computation, 2019, 15, 520-528.	5.3	40
5	Coreâ€“valence-separated coupled-cluster-singles-and-doubles complex-polarization-propagator approach to X-ray spectroscopies. Physical Chemistry Chemical Physics, 2020, 22, 2642-2647.	2.8	31
6	Coupled cluster study of the x-ray absorption spectra of formaldehyde derivatives at the oxygen, carbon, and fluorine K-edges. Journal of Chemical Physics, 2019, 151, 064107.	3.0	24
7	UV Absorption and Magnetic Circular Dichroism Spectra of Purine, Adenine, and Guanine: A Coupled Cluster Study in Vacuo and in Aqueous Solution. Journal of Chemical Theory and Computation, 2019, 15, 1242-1254.	5.3	24
8	Rovibrational and Temperature Effects in Theoretical Studies of NMR Parameters. New Developments in NMR, 2016, , 218-266.	0.1	23
9	RPA(D) and HRPA(D): Two new models for calculations of NMR indirect nuclear spinâ€“spin coupling constants. Journal of Computational Chemistry, 2018, 39, 2647-2666.	3.3	21
10	On the discrepancy between theory and experiment for the Fâ€“F spinâ€“spin coupling constant of difluoroethyne. Physical Chemistry Chemical Physics, 2012, 14, 16440.	2.8	19
11	On the convergence of zero-point vibrational corrections to nuclear shieldings and shielding anisotropies towards the complete basis set limit in water. Molecular Physics, 2017, 115, 144-160.	1.7	19
12	Picosecond timescale tracking of pentacene triplet excitons with chemical sensitivity. Communications Physics, 2019, 2, .	5.3	18
13	Noniterative Doubles Corrections to the Random Phase and Higher Random Phase Approximations: Singlet and Triplet Excitation Energies. Journal of Computational Chemistry, 2020, 41, 43-55.	3.3	17
14	Spinâ€orbit <scp>ZORA</scp> and fourâ€component <scp>D</scp>iracâ€“<scp>C</scp>oulomb estimation of relativistic corrections to isotropic nuclear shieldings and chemical shifts of noble gas dimers. Journal of Computational Chemistry, 2016, 37, 395-403.	3.3	14
15	On the convergence of the ccJ-pVXZ and pcJ-n basis sets in CCSD calculations of nuclear spinâ€“spin coupling constants: some difficult cases. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	14
16	SOPPA and CCSD vibrational corrections to NMR indirect spin-spin coupling constants of small hydrocarbons. AIP Conference Proceedings, 2015, , .	0.4	13
17	Spin adapted implementation of EOM-CCSD for triplet excited states: Probing intersystem crossings of acetylacetone at the carbon and oxygen K-edges. Journal of Chemical Physics, 2019, 151, 144107.	3.0	12
18	Magnetic circular dichroism spectra from resonant and damped coupled cluster response theory. Journal of Chemical Physics, 2020, 153, 114105.	3.0	10

#	Article	IF	Citations
19	NMR parameters of FNNF as a test for coupled-cluster methods: CCSDT shielding and CC3 spinâ€“spin coupling. Physical Chemistry Chemical Physics, 2020, 22, 21350-21359.	2.8	10
20	Benchmarking Correlated Methods for Frequency-Dependent Polarizabilities: Aromatic Molecules with the CC3, CCSD, CC2, SOPPA, SOPPA(CC2), and SOPPA(CCSD) Methods. Journal of Chemical Theory and Computation, 2020, 16, 3006-3018.	5.3	10