Rasmus Faber

List of Publications by Year
in descending order

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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	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
2	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
3	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
4	Magnetic circular dichroism spectra from resonant and damped coupled cluster response theory. Journal of Chemical Physics, 2020, 153, 114105.	3.0	10
5	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
6	Dalton Project: A Python platform for molecular- and electronic-structure simulations of complex systems. Journal of Chemical Physics, 2020, 152, 214115.	3.0	45
7	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
8	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
9	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
10	Picosecond timescale tracking of pentacene triplet excitons with chemical sensitivity. Communications Physics, 2019, 2, .	5.3	18
11	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
12	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
13	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
14	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
15	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
16	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
17	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
18	Rovibrational and Temperature Effects in Theoretical Studies of NMR Parameters. New Developments in NMR, 2016, , 218-266.	0.1	23

#	Article	IF	Citations
19	SOPPA and CCSD vibrational corrections to NMR indirect spin-spin coupling constants of small hydrocarbons. AIP Conference Proceedings, 2015, , .	0.4	13
20	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