Ajith Perera

List of Publications by Year
in descending order

57 papers	1,022 citations	430874 18 h-index	434195 31 g-index
57 all docs	57 docs citations	57 times ranked	958 citing authors

#	Article	IF	Citations
1	Benchmarking isotropic hyperfine coupling constants using (QTP) DFT functionals and coupled cluster theory. Journal of Chemical Physics, 2022, 156, 094107.	3.0	5
2	Reaction of Methylidyne with Ethane: The Câ€“C Insertion Is Unimportant. Journal of Physical Chemistry A, 2022, 126, 1966-1972.	2.5	1
3	The intermediate state approach for doubly excited dark states in EOM-coupled-cluster theory. Journal of Chemical Physics, 2022, 156, .	3.0	7
4	Examining fundamental and excitation gaps at the thermodynamic limit: A combined (QTP) DFT and coupled cluster study on trans-polyacetylene and polyacene. Journal of Chemical Physics, 2022, 156, .	3.0	3
5	Explicitly correlated Fock-space coupled-cluster singles and doubles method for (1,1), (0,2), and (2,0) sectors. Journal of Chemical Physics, 2021, 155, 014107.	3.0	3
6	Equation of motion coupled-cluster study of core excitation spectra II: Beyond the dipole approximation. Journal of Chemical Physics, 2021, 155, 094103.	3.0	15
7	Advanced concepts in electronic structure (ACES) software programs. Journal of Chemical Physics, 2020, 152, 184105.	3.0	24
8	A route to improving RPA excitation energies through its connection to equation-of-motion coupled cluster theory. Journal of Chemical Physics, 2020, 153, 234101.	3.0	7
9	Index of multi-determinantal and multi-reference character in coupled-cluster theory. Journal of Chemical Physics, 2020, 153, 234103.	3.0	17
10	Behind the success of modified coupled-cluster methods: addition by subtraction. Molecular Physics, 2019, 117, 2201-2216.	1.7	8
11	Equation of motion coupled-cluster for core excitation spectra: Two complementary approaches. Journal of Chemical Physics, 2019, 151, 164117.	3.0	34
12	Spin-orbit split ionized and electron-attached states using explicitly-correlated equation-of-motion coupled-cluster singles and doubles eigenvectors. Chemical Physics Letters, 2019, 730, 372-377.	2.6	6
13	Vertical valence ionization potential benchmarks from equation-of-motion coupled cluster theory and QTP functionals. Journal of Chemical Physics, 2019, 150, 074108.	3.0	46
14	Similarity-transformed equation-of-motion coupled-cluster singles and doubles method with spin-orbit effects for excited states. Journal of Chemical Physics, 2019, 151, 134110.	3.0	10
15	Explicitly-correlated double ionization potentials and double electron attachment equation-of-motion coupled cluster methods. Chemical Physics Letters, 2018, 692, 191-195.	2.6	11
16	Reference dependence of the two-determinant coupled-cluster method for triplet and open-shell singlet states of biradical molecules. Journal of Chemical Physics, 2018, 148, 164102.	3.0	6
17	Vibrational Characterization of Radical Ion Adducts between Imidazole and CO₂. Journal of Physical Chemistry A, 2018, 122, 3805-3810.	2.5	4
18	Spin-orbit splitted excited states using explicitly-correlated equation-of-motion coupled-cluster singles and doubles eigenvectors. Chemical Physics Letters, 2018, 698, 171-175.	2.6	4

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19	Low scaling EOM-CCSD and EOM-MBPT(2) method with natural transition orbitals. Journal of Chemical Physics, 2018, 149, 184103.	3.0	14
20	Long-range dispersion C6 coefficient for SF6 dimer: Experimental and theoretical study. Journal of Chemical Physics, 2018, 149, 124302.	3.0	1
21	Valence and charge-transfer optical properties for some SinCm(m,nâ€ˆâ‰ 12) clusters: Comparing TD-DFT, complete-basis-limit EOMCC, and benchmarks from spectroscopy. Journal of Chemical Physics, 2018, 148, 174309.	3.0	1
22	Explicitly-correlated coupled cluster method for long-range dispersion coefficients. Chemical Physics Letters, 2017, 672, 133-136.	2.6	2
23	Excited states from modified coupled cluster methods: Are they any better than EOM CCSD?. Journal of Chemical Physics, 2017, 146, 144104.	3.0	33
24	Towards core-excitation spectra in attosecond spectroscopy: A coupled-cluster study of ClF. Chemical Physics Letters, 2017, 683, 68-75.	2.6	12
25	Elementary reaction profile and chemical kinetics study of [C(1D)/(3P) + SiH4] with the CCSD(T) method. Chemical Physics Letters, 2017, 680, 61-68.	2.6	3
26	Benchmark coupled-cluster g-tensor calculations with full inclusion of the two-particle spin-orbit contributions. Journal of Chemical Physics, 2017, 146, 164104.	3.0	11
27	A note on the accuracy of KS-DFT densities. Journal of Chemical Physics, 2017, 147, 204103.	3.0	23
28	Single-reference coupled cluster theory for multi-reference problems. Journal of Chemical Physics, 2017, 147, 184101.	3.0	22
29	Excitation energies with spin-orbit couplings using equation-of-motion coupled-cluster singles and doubles eigenvectors. Journal of Chemical Physics, 2017, 147, 164118.	3.0	12
30	Explicitly correlated coupled-cluster theory for static polarizabilities. Journal of Chemical Physics, 2016, 145, 134104.	3.0	7
31	Assessing the distinguishable cluster approximation based on the triple bond-breaking in the nitrogen molecule. Journal of Chemical Physics, 2016, 144, 124117.	3.0	19
32	In honour of N. Yngve Ã–hrn: surveying proton cancer therapy reactions with Ã–hrn's electron nuclear dynamics method. Aqueous clusters radiolysis and DNA-base damage byÂprotonÂcollisions. Molecular Physics, 2015, 113, 297-313.	1.7	8
33	Approximating electronically excited states with equation-of-motion linear coupled-cluster theory. Journal of Chemical Physics, 2015, 143, 164103.	3.0	18
34	Coupled cluster geometries and energies of C20 carbon cluster isomers â€“ A new benchmark study. Chemical Physics Letters, 2015, 629, 76-80.	2.6	31
35	Spectroscopic analysis of diphosphatriazolate anion (P2N3â¯) by coupled-cluster methods as a step toward N5â¯. Chemical Physics Letters, 2015, 640, 68-71.	2.6	8
36	Structure and photochemistry of a bio-inspired model for photocatalytic H2O splitting: Improved calculations of the Sobolewski and Domcke's Chlorophyll-Imidazole-Benzoquinone model complex. Molecular Physics, 2014, 112, 863-867.	1.7	2

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37	Theoretical study of low-lying excited states of HSX (X = F, Cl, Br, I). Chemical Physics Letters, 2014, 602, 34-39.	2.6	1
38	Geometric Metastability in Molecules as a Way to Enhance Energy Storage. Advances in Quantum Chemistry, 2014, 69, 147-170.	0.8	2
39	Gas-Phase Synthesis of Boronylallene (H2CCCH(BO)) under Single Collision Conditions: A Crossed Molecular Beams and Computational Study. Journal of Physical Chemistry A, 2014, 118, 3810-3819.	2.5	6
40	Transition metal atomic multiplet states through the lens of single-reference coupled-cluster and the equation-of-motion coupled-cluster methods. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	11
41	Singletâ€“triplet separations of di-radicals treated by the DEA/DIP-EOM-CCSD methods. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	24
42	Benchmarking for Perturbative Triple-Excitations in EE-EOM-CC Methods. Journal of Physical Chemistry A, 2013, 117, 2569-2579.	2.5	63
43	Benchmark Studies on the Building Blocks of DNA. 3. Watsonâ€“Crick and Stacked Base Pairs. Journal of Physical Chemistry A, 2013, 117, 3149-3157.	2.5	37
44	A Crossed Molecular Beam and Ab-Initio Investigation of the Reaction of Boron Monoxide (BO;) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 47 Physical Chemistry A, 2013, 117, 11794-11807.	2.5	13
45	Massively parallel implementations of coupled-cluster methods for electron spin resonance spectra. I. Isotropic hyperfine coupling tensors in large radicals. Journal of Chemical Physics, 2013, 139, 174103.	3.0	16
46	Benchmark Studies on the Building Blocks of DNA. 2. Effect of Biological Environment on the Electronic Excitation Spectrum of Nucleobases. Journal of Physical Chemistry A, 2012, 116, 8851-8860.	2.5	35
47	Benchmark Studies on the Building Blocks of DNA. 1. Superiority of Coupled Cluster Methods in Describing the Excited States of Nucleobases in the Franckâ€“Condon Region. Journal of Physical Chemistry A, 2012, 116, 6702-6710.	2.5	91
48	Increasing the applicability of DFT I: Non-variational correlation corrections from Hartreeâ€“Fock DFT for predicting transition states. Chemical Physics Letters, 2012, 524, 10-15.	2.6	72
49	Multireference coupled-cluster theory: The easy way. Journal of Chemical Physics, 2011, 134, 114108.	3.0	114
50	Software design of ACES III with the super instruction architecture. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 895-901.	14.6	54
51	Ab initio simulation of UV/vis absorption spectra for atmospheric modeling: method design for medium-sized molecules. Physical Chemistry Chemical Physics, 2010, 12, 9726.	2.8	4
52	What made possible the accurate calculations of NMR spinâ€“spin coupling constants?. Molecular Physics, 2010, 108, 3017-3025.	1.7	12
53	An ab initio study of the (H[sub 2]O)[sub 20]H[sup +] and (H[sub 2]O)[sub 21]H[sup +] water clusters. Journal of Chemical Physics, 2009, 131, 104313.	3.0	28
54	Predictive Quantum Chemistry: A Step Toward â€œChemistry Without Test Tubesâ€• AIP Conference Proceedings, 2007, , .	0.4	0

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55	New massively parallel linear-response coupled-cluster module in ACES III: application to static polarisabilities of closed-shell molecules and oligomers and of open-shell radicals. Molecular Physics, 0, , 1-15.	1.7	1
56	The reaction of Hâ€‰+â€‰CH2O: addition vs. abstraction. Molecular Physics, 0, , e1928315.	1.7	0
57	Introduction to the John Stanton special issue. Molecular Physics, 0, , .	1.7	0