

Ajith Perera

List of Publications by Year in descending order

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57
papers

1,022
citations

430874

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all docs

57
docs citations

57
times ranked

958
citing authors

#	ARTICLE	IF	CITATIONS
1	Multireference coupled-cluster theory: The easy way. <i>Journal of Chemical Physics</i> , 2011, 134, 114108.	3.0	114
2	Benchmark Studies on the Building Blocks of DNA. 1. Superiority of Coupled Cluster Methods in Describing the Excited States of Nucleobases in the Franck-Condon Region. <i>Journal of Physical Chemistry A</i> , 2012, 116, 6702-6710.	2.5	91
3	Increasing the applicability of DFT I: Non-variational correlation corrections from Hartree-Fock DFT for predicting transition states. <i>Chemical Physics Letters</i> , 2012, 524, 10-15.	2.6	72
4	Benchmarking for Perturbative Triple-Excitations in EE-EOM-CC Methods. <i>Journal of Physical Chemistry A</i> , 2013, 117, 2569-2579.	2.5	63
5	Software design of ACES III with the super instruction architecture. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2011, 1, 895-901.	14.6	54
6	Vertical valence ionization potential benchmarks from equation-of-motion coupled cluster theory and QTP functionals. <i>Journal of Chemical Physics</i> , 2019, 150, 074108.	3.0	46
7	Benchmark Studies on the Building Blocks of DNA. 3. Watson-Crick and Stacked Base Pairs. <i>Journal of Physical Chemistry A</i> , 2013, 117, 3149-3157.	2.5	37
8	Benchmark Studies on the Building Blocks of DNA. 2. Effect of Biological Environment on the Electronic Excitation Spectrum of Nucleobases. <i>Journal of Physical Chemistry A</i> , 2012, 116, 8851-8860.	2.5	35
9	Equation of motion coupled-cluster for core excitation spectra: Two complementary approaches. <i>Journal of Chemical Physics</i> , 2019, 151, 164117.	3.0	34
10	Excited states from modified coupled cluster methods: Are they any better than EOM CCSD?. <i>Journal of Chemical Physics</i> , 2017, 146, 144104.	3.0	33
11	Coupled cluster geometries and energies of C ₂₀ carbon cluster isomers – A new benchmark study. <i>Chemical Physics Letters</i> , 2015, 629, 76-80.	2.6	31
12	An ab initio study of the (H ₂ O) ₂₀ H ⁺ and (H ₂ O) ₂₁ H ⁺ water clusters. <i>Journal of Chemical Physics</i> , 2009, 131, 104313.	3.0	28
13	Singlet-triplet separations of di-radicals treated by the DEA/DIP-EOM-CCSD methods. <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1.	1.4	24
14	Advanced concepts in electronic structure (ACES) software programs. <i>Journal of Chemical Physics</i> , 2020, 152, 184105.	3.0	24
15	A note on the accuracy of KS-DFT densities. <i>Journal of Chemical Physics</i> , 2017, 147, 204103.	3.0	23
16	Single-reference coupled cluster theory for multi-reference problems. <i>Journal of Chemical Physics</i> , 2017, 147, 184101.	3.0	22
17	Assessing the distinguishable cluster approximation based on the triple bond-breaking in the nitrogen molecule. <i>Journal of Chemical Physics</i> , 2016, 144, 124117.	3.0	19
18	Approximating electronically excited states with equation-of-motion linear coupled-cluster theory. <i>Journal of Chemical Physics</i> , 2015, 143, 164103.	3.0	18

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19	Index of multi-determinantal and multi-reference character in coupled-cluster theory. Journal of Chemical Physics, 2020, 153, 234103.	3.0	17
20	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
21	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
22	Low scaling EOM-CCSD and EOM-MBPT(2) method with natural transition orbitals. Journal of Chemical Physics, 2018, 149, 184103.	3.0	14
23	A Crossed Molecular Beam and Ab-Initio Investigation of the Reaction of Boron Monoxide (BO); Tj ETQq1 1 0.784314 rgBT /Overlock 10 Physical Chemistry A, 2013, 117, 11794-11807.	2.5	13
24	What made possible the accurate calculations of NMR spin-spin coupling constants?. Molecular Physics, 2010, 108, 3017-3025.	1.7	12
25	Towards core-excitation spectra in attosecond spectroscopy: A coupled-cluster study of ClF. Chemical Physics Letters, 2017, 683, 68-75.	2.6	12
26	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
27	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
28	Benchmark coupled-cluster $\langle i g \rangle$ -tensor calculations with full inclusion of the two-particle spin-orbit contributions. Journal of Chemical Physics, 2017, 146, 164104.	3.0	11
29	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
30	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
31	In honour of N. Yngve Åhrn: surveying proton cancer therapy reactions with Åhrn's electron nuclear dynamics method. Aqueous clusters radiolysis and DNA-base damage by Åproton Åcollisions. Molecular Physics, 2015, 113, 297-313.	1.7	8
32	Spectroscopic analysis of diphosphatriazolate anion (P2N3 $\hat{\sim}$) by coupled-cluster methods as a step toward N5 $\hat{\sim}$. Chemical Physics Letters, 2015, 640, 68-71.	2.6	8
33	Behind the success of modified coupled-cluster methods: addition by subtraction. Molecular Physics, 2019, 117, 2201-2216.	1.7	8
34	Explicitly correlated coupled-cluster theory for static polarizabilities. Journal of Chemical Physics, 2016, 145, 134104.	3.0	7
35	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
36	The intermediate state approach for doubly excited dark states in EOM-coupled-cluster theory. Journal of Chemical Physics, 2022, 156, .	3.0	7

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37	Gas-Phase Synthesis of Boronallene (H ₂ CCCH(BO)) under Single Collision Conditions: A Crossed Molecular Beams and Computational Study. <i>Journal of Physical Chemistry A</i> , 2014, 118, 3810-3819.	2.5	6
38	Reference dependence of the two-determinant coupled-cluster method for triplet and open-shell singlet states of biradical molecules. <i>Journal of Chemical Physics</i> , 2018, 148, 164102.	3.0	6
39	Spin-orbit split ionized and electron-attached states using explicitly-correlated equation-of-motion coupled-cluster singles and doubles eigenvectors. <i>Chemical Physics Letters</i> , 2019, 730, 372-377.	2.6	6
40	Benchmarking isotropic hyperfine coupling constants using (QTP) DFT functionals and coupled cluster theory. <i>Journal of Chemical Physics</i> , 2022, 156, 094107.	3.0	5
41	Ab initio simulation of UV/vis absorption spectra for atmospheric modeling: method design for medium-sized molecules. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 9726.	2.8	4
42	Vibrational Characterization of Radical Ion Adducts between Imidazole and CO ₂ . <i>Journal of Physical Chemistry A</i> , 2018, 122, 3805-3810.	2.5	4
43	Spin-orbit splitted excited states using explicitly-correlated equation-of-motion coupled-cluster singles and doubles eigenvectors. <i>Chemical Physics Letters</i> , 2018, 698, 171-175.	2.6	4
44	Elementary reaction profile and chemical kinetics study of [C(1D)/(3P) + SiH ₄] with the CCSD(T) method. <i>Chemical Physics Letters</i> , 2017, 680, 61-68.	2.6	3
45	Explicitly correlated Fock-space coupled-cluster singles and doubles method for (1,1), (0,2), and (2,0) sectors. <i>Journal of Chemical Physics</i> , 2021, 155, 014107.	3.0	3
46	Examining fundamental and excitation gaps at the thermodynamic limit: A combined (QTP) DFT and coupled cluster study on <i>trans</i> -polyacetylene and polyacene. <i>Journal of Chemical Physics</i> , 2022, 156, .	3.0	3
47	Structure and photochemistry of a bio-inspired model for photocatalytic H ₂ O splitting: Improved calculations of the Sobolewski and Domcke's Chlorophyll-Imidazole-Benzoquinone model complex. <i>Molecular Physics</i> , 2014, 112, 863-867.	1.7	2
48	Geometric Metastability in Molecules as a Way to Enhance Energy Storage. <i>Advances in Quantum Chemistry</i> , 2014, 69, 147-170.	0.8	2
49	Explicitly-correlated coupled cluster method for long-range dispersion coefficients. <i>Chemical Physics Letters</i> , 2017, 672, 133-136.	2.6	2
50	Theoretical study of low-lying excited states of HSX (X = F, Cl, Br, I). <i>Chemical Physics Letters</i> , 2014, 602, 34-39.	2.6	1
51	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. <i>Molecular Physics</i> , 0, , 1-15.	1.7	1
52	Long-range dispersion C ₆ coefficient for SF ₆ dimer: Experimental and theoretical study. <i>Journal of Chemical Physics</i> , 2018, 149, 124302.	3.0	1
53	Valence and charge-transfer optical properties for some Si _n C _m ($n \le 12$) clusters: Comparing TD-DFT, complete-basis-limit EOMCC, and benchmarks from spectroscopy. <i>Journal of Chemical Physics</i> , 2018, 148, 174309.	3.0	1
54	Reaction of Methylidyne with Ethane: The C=C Insertion Is Unimportant. <i>Journal of Physical Chemistry A</i> , 2022, 126, 1966-1972.	2.5	1

#	ARTICLE	IF	CITATIONS
55	Predictive Quantum Chemistry: A Step Toward "Chemistry Without Test Tubes", AIP Conference Proceedings, 2007, , .	0.4	0
56	The reaction of H+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