Achintya Kumar Dutta

List of Publications by Year
in descending order

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Version: 2024-02-01

46	919	516710	477307
papers	citations	16 h-index	29 g-index

47	47	47	697
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A similarity transformed second-order approximate coupled cluster method for the excited states: Theory, implementation, and benchmark. Journal of Chemical Physics, 2022, 156, 014110.	3.0	1
2	The performance of approximate<scp>EOMâ€CCSD</scp>for ionization potential and electron affinity of genetic material subunits: A benchmark investigation. International Journal of Quantum Chemistry, 2022, 122, .	2.0	4
3	A reduced cost four-component relativistic coupled cluster method based on natural spinors. Journal of Chemical Physics, 2022, 156, .	3.0	6
4	Pair Natural Orbital Equation-of-Motion Coupled-Cluster Method for Core Binding Energies: Theory, Implementation, and Benchmark. Journal of Chemical Theory and Computation, 2022, 18, 4660-4673.	5.3	2
5	Electron Attachment to Cytosine: The Role of Water. Journal of Physical Chemistry A, 2021, 125, 4683-4694.	2.5	9
6	An efficient Fock space multi-reference coupled cluster method based on natural orbitals: Theory, implementation, and benchmark. Journal of Chemical Physics, 2021, 155, 014105.	3.0	4
7	Efficient EOM-CC-based Protocol for the Calculation of Electron Affinity of Solvated Nucleobases: Uracil as a Case Study. Journal of Chemical Theory and Computation, 2021, 17, 105-116.	5.3	16
8	Doorway Mechanism for Electron Attachment Induced DNA Strand Breaks. Journal of Physical Chemistry Letters, 2021, 12, 10380-10387.	4.6	15
9	A Coreâ€"Valence Separated Similarity Transformed EOM-CCSD Method for Core-Excitation Spectra. Journal of Chemical Theory and Computation, 2021, 17, 7428-7446.	5.3	9
10	Solvation effect on the vertical ionization energy of adenineâ€thymine base pair: From microhydration to bulk. International Journal of Quantum Chemistry, 2020, 120, e26127.	2.0	4
11	A new density for transition properties within the similarity transformed equation of motion approach. Molecular Physics, 2020, 118, e1818858.	1.7	3
12	Water mediated electron attachment to nucleobases: Surface-bound vs bulk solvated electrons. Journal of Chemical Physics, 2020, 153, 044305.	3.0	15
13	A Multilayer Approach to the Equation of Motion Coupled-Cluster Method for the Electron Affinity. Journal of Physical Chemistry A, 2020, 124, 3947-3962.	2.5	12
14	Interactions of Solvated Electrons with Nucleobases: The Effect of Base Pairing. ChemPhysChem, 2020, 21, 1019-1027.	2.1	11
15	Ruthenium-Chelated Non-Innocent Bis(heterocyclo)methanides: A Mimicked Î²-Diketiminate. Inorganic Chemistry, 2019, 58, 11458-11469.	4.0	30
16	A domain-based local pair natural orbital implementation of the equation of motion coupled cluster method for electron attached states. Journal of Chemical Physics, 2019, 150, 164123.	3.0	57
17	Multilayer Approach to the IP-EOM-DLPNO-CCSD Method: Theory, Implementation, and Application. Journal of Chemical Theory and Computation, 2019, 15, 2265-2277.	5.3	21
18	Electron Attachment to DNA Base Pairs: An Interplay of Dipole- and Valence-Bound States. Journal of Physical Chemistry A, 2019, 123, 10131-10138.	2.5	21

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19	Accurate Ionization Potentials, Electron Affinities and Electronegativities of Single-Walled Carbon Nanotubes by State-of-the-Art Local Coupled-Cluster Theory. Bulletin of the Chemical Society of Japan, 2019, 92, 170-174.	3.2	3
20	Bound anionic states of DNA and RNA nucleobases: An EOMâ€CCSD investigation. International Journal of Quantum Chemistry, 2019, 119, e25875.	2.0	12
21	Lower scaling approximation to EOMâ€CCSD: A critical assessment of the ionization problem. International Journal of Quantum Chemistry, 2018, 118, e25594.	2.0	18
22	Accelerating the coupled-cluster singles and doubles method using the chain-of-sphere approximation. Molecular Physics, 2018, 116, 1428-1434.	1.7	19
23	Exploring the Accuracy of a Low Scaling Similarity Transformed Equation of Motion Method for Vertical Excitation Energies. Journal of Chemical Theory and Computation, 2018, 14, 72-91.	5.3	89
24	Systematic Highâ€Accuracy Prediction of Electron Affinities for Biological Quinones. Journal of Computational Chemistry, 2018, 39, 2439-2451.	3.3	9
25	A near-linear scaling equation of motion coupled cluster method for ionized states. Journal of Chemical Physics, 2018, 148, 244101.	3.0	51
26	Automatic active space selection for the similarity transformed equations of motion coupled cluster method. Journal of Chemical Physics, 2017, 146, 074103.	3.0	53
27	A simple scheme for calculating approximate transition moments within the equation of motion expectation value formalism. Journal of Chemical Physics, 2017, 146, 214111.	3.0	10
28	Resolution of the Identity and Cholesky Representation of EOM-MP2 Approximation: Implementation, Accuracy and Efficiency. Journal of Chemical Sciences, 2017, 129, 1611-1626.	1.5	5
29	Towards a pair natural orbital coupled cluster method for excited states. Journal of Chemical Physics, 2016, 145, 034102.	3.0	115
30	Speeding up equation of motion coupled cluster theory with the chain of spheres approximation. Journal of Chemical Physics, 2016, 144, 034102.	3.0	62
31	Electron Detachment and Subsequent Structural Changes of Water Clusters. Journal of Physical Chemistry A, 2016, 120, 1065-1073.	2.5	5
32	Electron attachment to DNA and RNA nucleobases: An EOMCC investigation. International Journal of Quantum Chemistry, 2015, 115, 753-764.	2.0	16
33	EOMIP-CCSD(2)*: An Efficient Method for the Calculation of Ionization Potentials. Journal of Chemical Theory and Computation, 2015, 11, 2461-2472.	5.3	25
34	A new scheme for perturbative triples correction to (0,1) sector of Fock space multi-reference coupled cluster method: Theory, implementation, and examples. Journal of Chemical Physics, 2015, 142, 044113.	3.0	7
35	Perturbative order analysis of the similarity transformed Hamiltonian in Fock-space coupled cluster theory: difference energy and electric response properties. Molecular Physics, 2015, 113, 2046-2060.	1.7	1
36	Ground state of naphthyl cation: Singlet or triplet?. Journal of Chemical Physics, 2014, 140, 114312.	3.0	2

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37	Structure, Stability, and Properties of the Trans Peroxo Nitrate Radical: The Importance of Nondynamic Correlation. Journal of Physical Chemistry A, 2014, 118, 1350-1362.	2.5	3
38	Partitioned EOMEA-MBPT(2): An Efficient N⁵ Scaling Method for Calculation of Electron Affinities. Journal of Chemical Theory and Computation, 2014, 10, 1923-1933.	5.3	30
39	Intermediate Hamiltonian Fock Space Multireference Coupled Cluster Approach to Core Excitation Spectra. Journal of Chemical Theory and Computation, 2014, 10, 3656-3668.	5.3	29
40	Excited state geometry optimisation using Fock-space multi-reference coupled cluster method. Molecular Physics, 2014, 112, 2884-2891.	1.7	0
41	Performance of the EOMIP-CCSD(2) Method for Determining the Structure and Properties of Doublet Radicals: A Benchmark Investigation. Journal of Chemical Theory and Computation, 2013, 9, 4313-4331.	5.3	35
42	Perturbative approximations to single and double spin flip equation of motion coupled cluster singles doubles methods. Journal of Chemical Physics, 2013, 139, 124116.	3.0	28
43	Conformational modulation of Antâ€“Pro oligomers using chirality alteration of proline residues. Organic and Biomolecular Chemistry, 2012, 10, 8426.	2.8	13
44	Friedelâ€“Crafts Acylation Reactions Using Esters. European Journal of Organic Chemistry, 2012, 2012, 6841-6845.	2.4	14
45	Extended coupled cluster for Raman and infrared spectra of small molecules. Chemical Physics, 2012, 403, 25-32.	1.9	8
46	NOx Catalyzed Pathway of Stratospheric Ozone Depletion: A Coupled Cluster Investigation. Journal of Chemical Theory and Computation, 2012, 8, 1895-1901.	5.3	4