Nayana Vaval

List of Publications by Year
in descending order

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80	1,107	394421	501196
papers	citations	19	28
		h-index	g-index

81	81	81	592
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Decay Processes in Cationic Alkali Metals in Microsolvated Clusters: A Complex Absorbing Potential Based Equation-of-Motion Coupled Cluster Investigation. Journal of Chemical Theory and Computation, 2022, 18, 807-816.	5.3	4
2	Interatomic Coulombic decay in Neonâ€“Helium cluster: a complex absorbing potential based equation-of-motion coupled cluster investigation. Molecular Physics, 2021, 119, e1884300.	1.7	1
3	Resonance study: Effect of partial triples excitation using complex absorbing potentialâ€based Fockâ€space multiâ€reference coupled cluster. International Journal of Quantum Chemistry, 2021, 121, e26738.	2.0	1
4	Negative Ion Resonance States: The Fock-Space Coupled-Cluster Way. Journal of Physical Chemistry A, 2020, 124, 10407-10421.	2.5	5
5	Electronic structure parameter of nuclear magnetic quadrupole moment interaction in metal monofluorides. Journal of Chemical Physics, 2020, 153, 184306.	3.0	9
6	Relativistic double-ionization equation-of-motion coupled-cluster method: Application to low-lying doubly ionized states. Journal of Chemical Physics, 2020, 152, 104302.	3.0	1
7	Role of electron correlation in the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="script">P</mml:mi><mml:mo>,</mml:mo><mml:mi mathvariant="script">T</mml:mi></mml:mrow></mml:math> -odd effects of CdH: A relativistic coupled-cluster investigation. Physical Review A, 2020, 101, .	2.5	3
8	Shape resonance of sulphur dioxide anion excited states using the CAP-CIP-FSMRCCSD method. Molecular Physics, 2020, 118, .	1.7	6
9	Relativistic coupled-cluster study of BaF in search of $oldsymbol{mathcal{CP}}$ violation. Journal of Physics B: Atomic, Molecular and Optical Physics, 2020, 53, 135102.	1.5	7
10	Nuclear parity- and time-reversal-symmetry violation in the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mmultiscripts><mml:mi>HgH</mml:mi><mml:mprescripts /><mml:none /><mml:mn>201</mml:mn></mml:mmultiscripts></mml:math> molecule. Physical Review A, 2019, 99, .	2.5	7
11	Relativistic coupled-cluster investigation of parity (P) and time-reversal (T) symmetry violations in HgF. Journal of Chemical Physics, 2019, 150, 084304.	3.0	8
12	Lower scaling approximation to EOMâ€CCSD: A critical assessment of the ionization problem. International Journal of Quantum Chemistry, 2018, 118, e25594.	2.0	18
13	Correlation trends in the magnetic hyperfine structure of atoms: A relativistic coupled-cluster case study. Physical Review A, 2018, 98, .	2.5	7
14	Auger decay rates of core hole states using equation of motion coupled cluster method. Chemical Physics, 2017, 482, 160-164.	1.9	6
15	Electronâ€“nucleus scalarâ€“pseudoscalar interaction in PbF: Z-vector study in the relativistic coupled-cluster framework. Molecular Physics, 2017, 115, 2807-2812.	1.7	6
16	Relativistic equation-of-motion coupled-cluster method using open-shell reference wavefunction: Application to ionization potential. Journal of Chemical Physics, 2016, 145, 074110.	3.0	18
17	Search for parity and time reversal violating effects in HgH: Relativistic coupled-cluster study. Journal of Chemical Physics, 2016, 144, 124307.	3.0	19
18	Relativistic coupled-cluster study of RaF as a candidate for the parity- and time-reversal-violating interaction. Physical Review A, 2016, 93, .	2.5	33

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19	Relativistic equation-of-motion coupled-cluster method for the electron attachment problem. Computational and Theoretical Chemistry, 2016, 1076, 94-100.	2.5	13
20	Lifetime of inner-shell hole states of Ar (2p) and Kr (3d) using equation-of-motion coupled cluster method. Journal of Chemical Physics, 2015, 143, 024305.	3.0	8
21	Calculation of P,T-odd interaction constant of PbF using Z-vector method in the relativistic coupled-cluster framework. Journal of Chemical Physics, 2015, 143, 084119.	3.0	16
22	Electron attachment to DNA and RNA nucleobases: An EOMCC investigation. International Journal of Quantum Chemistry, 2015, 115, 753-764.	2.0	16
23	A relativistic equation-of-motion coupled-cluster investigation of the trends of single and double ionization potentials in the He and Be isoelectronic systems. Journal of Physics B: Atomic, Molecular and Optical Physics, 2015, 48, 115009.	1.5	5
24	Implementation of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Z</mml:mi></mml:math>-vector method in the relativistic-coupled-cluster framework to calculate first-order energy derivatives: Application to the SrF molecule. Physical Review A, 2015, 91, .	2.5	19
25	Systematic comparison of DFT and CCSD dipole moments, polarizabilities and hyperpolarizabilities. Chemical Physics Letters, 2015, 635, 168-173.	2.6	17
26	Relativistic extended-coupled-cluster method for the magnetic hyperfine structure constant. Physical Review A, 2015, 91, .	2.5	9
27	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
28	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
29	Relativistic equation-of-motion coupled-cluster method for the ionization problem: Application to molecules. Physical Review A, 2014, 90, .	2.5	14
30	Complex absorbing potential based equation-of-motion coupled cluster method for the potential energy curve of $ext{CO}_{2}^{-}$CO2â^' anion. Journal of Chemical Physics, 2014, 141, 164113.	3.0	19
31	Relativistic equation-of-motion coupled-cluster method: Application to closed-shell atomic systems. Physical Review A, 2014, 89, .	2.5	27
32	Geometry-dependent lifetime of Interatomic coulombic decay using equation-of-motion coupled cluster method. Journal of Chemical Physics, 2014, 141, 234108.	3.0	16
33	Electronic transition dipole moment: A semiâ€biorthogonal approach within valence universal coupled cluster framework. International Journal of Quantum Chemistry, 2014, 114, 1212-1219.	2.0	5
34	Ground state of naphthyl cation: Singlet or triplet?. Journal of Chemical Physics, 2014, 140, 114312.	3.0	2
35	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
36	Extended coupled cluster method for potential energy surface: A decoupled approach. Chemical Physics Letters, 2014, 612, 209-213.	2.6	1

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37	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
38	Interatomic Coulombic decay in (n= 2â€“3) clusters using CAP/EOM-CCSD method. Molecular Physics, 2014, 112, 669-673.	1.7	20
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	Relativistic equation-of-motion coupled-cluster method for the double-ionization potentials of closed-shell atoms. Physical Review A, 2014, 90, .	2.5	16
41	Multipole moments using extended coupled cluster method. Chemical Physics Letters, 2013, 568-569, 170-175.	2.6	1
42	Study of interatomic Coulombic decay of Ne(H2O)n (n = 1,3) clusters using equation-of-motion coupled-cluster method. Journal of Chemical Physics, 2013, 139, 064112.	3.0	18
43	Fock space multireference coupled cluster theory: Study of shape resonance. International Journal of Quantum Chemistry, 2013, 113, 1690-1695.	2.0	4
44	CAP/EOM-CCSD method for the study of potential curves of resonant states. Physical Chemistry Chemical Physics, 2013, 15, 17915.	2.8	30
45	Extended coupled cluster through nth perturbation order for molecular response properties: A comparative study. Chemical Physics, 2013, 417, 45-51.	1.9	0
46	Polarizability of few electron quantum dots: Extended coupled-cluster response approach. Chemical Physics Letters, 2013, 555, 263-267.	2.6	6
47	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
48	Electronic transition dipole moments and dipole oscillator strengths within Fock-space multi-reference coupled cluster framework: An efficient and novel approach. Journal of Chemical Physics, 2013, 138, 094108.	3.0	22
49	A Lagrange multiplier approach for excited state properties through intermediate Hamiltonian formulation of Fock space multireference coupled-cluster theory. Journal of Chemical Physics, 2013, 139, 074108.	3.0	6
50	Equation-of-motion coupled-cluster method for the study of shape resonance. Journal of Chemical Physics, 2012, 136, 234110.	3.0	54
51	Extended coupled cluster for Raman and infrared spectra of small molecules. Chemical Physics, 2012, 403, 25-32.	1.9	8
52	NOx Catalyzed Pathway of Stratospheric Ozone Depletion: A Coupled Cluster Investigation. Journal of Chemical Theory and Computation, 2012, 8, 1895-1901.	5.3	4
53	Fock-space multi-reference coupled-cluster response with the effect of triples on dipole moment of ClO and SF radicals#. Journal of Chemical Sciences, 2012, 124, 223-232.	1.5	3
54	Constrained variational approach for energy derivatives in Intermediate Hamiltonian Fock-space coupled-cluster theory. Chemical Physics, 2012, 401, 45-49.	1.9	1

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55	Effect of Triples to Dipole Moments in Fock-Space Multireference Coupled Cluster Method. Journal of Chemical Theory and Computation, 2011, 7, 876-883.	5.3	5
56	First- and second-order electrical properties computed at the FSMRCCSD level for excited states of closed-shell molecules using the constrained-variational approach. Journal of Chemical Physics, 2009, 131, 024102.	3.0	30
57	Magnetizability of doublet radicals using Fock space multiâ€reference coupled cluster method. International Journal of Quantum Chemistry, 2009, 109, 2191-2198.	2.0	2
58	Ab initio lifetimes in the interatomic Coulombic decay of neon clusters computed with propagators. Journal of Chemical Physics, 2007, 126, 164110.	3.0	58
59	Constrained variational response to Fock-space multi-reference coupled-cluster theory: Some pilot applications. Computational and Theoretical Chemistry, 2006, 768, 91-96.	1.5	14
60	Analytically continued Fock space multi-reference coupled-cluster theory: Application to the shape resonance. Chemical Physics, 2006, 329, 283-289.	1.9	12
61	Electronic Spectra and Ionization Potentials of Halogen Oxides Using the Fock Space Coupled-Cluster Method. Collection of Czechoslovak Chemical Communications, 2005, 70, 851-863.	1.0	2
62	Electric properties of molecules using stationary coupled-cluster method. Journal of Computational Methods in Sciences and Engineering, 2004, 4, 721-736.	0.2	0
63	Fock space multireference coupled cluster calculations based on an underlying bivariational self-consistent field on Auger and shape resonances. Journal of Chemical Physics, 2004, 120, 67-72.	3.0	27
64	Extended coupled-cluster approach for magnetizabilities of small molecules. Chemical Physics Letters, 2004, 387, 442-447.	2.6	10
65	A fully relaxed extended coupled-cluster approach for molecular properties. Chemical Physics Letters, 2004, 398, 194-200.	2.6	9
66	Density functional study on the structure and stability of positive iron rare-gas complexes, (X=Ar, Xe;) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	1.9	1
67	Extended Coupled Cluster Approach for Molecular Properties: Study of H2O and HF Complexes. International Journal of Molecular Sciences, 2001, 2, 89-102.	4.1	14
68	Study of constant term for electronâ€“molecule scattering: F2, H2CO and H2O target examples. Chemical Physics Letters, 2001, 345, 319-324.	2.6	3
69	Molecular properties using bi-orthogonal functional: a de-coupled scheme. Chemical Physics Letters, 2000, 318, 168-172.	2.6	10
70	Multireference coupled cluster based analytic response approach for evaluating molecular properties: Some pilot results. Journal of Chemical Physics, 1999, 110, 2316-2322.	3.0	36
71	Adiabatic states of ozone using Fock space multireference coupled cluster method. Journal of Chemical Physics, 1999, 111, 4051-4055.	3.0	18
72	Molecular property calculations for excited states using a multireference coupled-cluster approach. Chemical Physics Letters, 1999, 300, 125-130.	2.6	16

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73	An extended coupled-cluster functional for molecular properties: study of an analytical and numerical approach. Chemical Physics Letters, 1998, 295, 189-194.	2.6	13
74	Fock space multireference coupled cluster theory: noniterative inclusion of triples for excitation energies. Theoretical Chemistry Accounts, 1998, 99, 100-105.	1.4	54
75	ANALYTIC COUPLED CLUSTER BASED RESPONSE APPROACH USING MULTIDETERMINANTAL MODEL SPACE. Recent Advances in Computational, 1997, , 255-273.	0.8	0
76	Stationary coupled-cluster approaches to molecular properties: A comparative study. Physical Review A, 1996, 54, 250-258.	2.5	30
77	Stationary multideterminantal coupled-cluster response. Physical Review A, 1994, 49, 1623-1628.	2.5	4
78	Nonlinear molecular properties using biorthogonal response approach. Journal of Chemical Physics, 1994, 101, 4914-4919.	3.0	37
79	Stationary coupled cluster response: Role of cubic terms in molecular properties. Journal of Chemical Sciences, 1994, 106, 387-392.	1.5	4
80	Fock-space multireference coupled-cluster theory. fourth-order corrections to the ionization potential. Chemical Physics Letters, 1993, 209, 292-298.	2.6	30