Sourav Pal

List of Publications by Year in descending order

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187 papers	4,436 citations	117625 34 h-index	149698 56 g-index
191 all docs	191 docs citations	191 times ranked	2336 citing authors

#	Article	IF	Citations
1	Use of Cluster Expansion Methods in the Open-Shell Correlation Problem. Advances in Quantum Chemistry, 1989, 20, 291-373.	0.8	353
2	Molecular applications of multireference coupledâ€cluster methods using an incomplete model space: Direct calculation of excitation energies. Journal of Chemical Physics, 1988, 88, 4357-4366.	3.0	228
3	Multireference coupled-cluster methods using an incomplete model space: Application to ionization potentials and excitation energies of formaldehyde. Chemical Physics Letters, 1987, 137, 273-278.	2.6	188
4	Critical Study of Local Reactivity Descriptors for Weak Interactions:â€‰ Qualitative and Quantitative Analysis of Adsorption of Molecules in the Zeolite Lattice. Journal of the American Chemical Society, 2000, 122, 4145-4153.	13.7	118
5	On non-negativity of Fukui function indices. II. Journal of Chemical Physics, 2000, 113, 1372-1379.	3.0	110
6	Mulliken population analysis based evaluation of condensed Fukui function indices using fractional molecular charge. Journal of Chemical Physics, 2001, 115, 2901-2907.	3.0	92
7	Principle of maximum hardness: an accurate ab initio study. The Journal of Physical Chemistry, 1993, 97, 4404-4406.	2.9	91
8	Defect Induced Performance Enhancement of Monolayer MoS₂ for Li- and Na-Ion Batteries. Journal of Physical Chemistry C, 2019, 123, 21852-21865.	3.1	78
9	Aromaticity and antiaromaticity of LixAl4clusters: Ring current patterns versus electron counting. Physical Chemistry Chemical Physics, 2004, 6, 285-288.	2.8	76
10	Use of a size-consistent energy functional in many electron theory for closed shells. Theoretica Chimica Acta, 1983, 62, 523-536.	0.8	60
11	Multireference coupledâ€cluster method: Ionization potentials and excitation energies for ketene and diazomethane. Journal of Chemical Physics, 1989, 90, 3214-3220.	3.0	57
12	Multireference coupled-cluster response approach for the calculation of static properties. Physical Review A, 1989, 39, 39-42.	2.5	56
13	Stateâ€selective multireference coupledâ€cluster theory: In pursuit of property calculation. Journal of Chemical Physics, 1996, 104, 6582-6589.	3.0	56
14	Fock space multireference coupled cluster theory: noniterative inclusion of triples for excitation energies. Theoretical Chemistry Accounts, 1998, 99, 100-105.	1.4	54
15	Equation-of-motion coupled-cluster method for the study of shape resonance. Journal of Chemical Physics, 2012, 136, 234110.	3.0	54
16	Study of Local Hardâ^'Soft Acidâ^'Base Principle to Multiple-Site Interactions. Journal of Physical Chemistry A, 2002, 106, 5737-5744.	2.5	52
17	Calculation of vibrational energy of molecule using coupled cluster linear response theory in bosonic representation: Convergence studies. Journal of Chemical Physics, 2008, 129, 134111.	3.0	52
18	Strategic Preparation of Efficient and Durable NiCo Alloy Supported Nâ€Ðoped Porous Graphene as an Oxygen Evolution Electrocatalyst: A Theoretical and Experimental Investigation. Advanced Materials Interfaces, 2016, 3, 1600532.	3.7	50

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19	Intermolecular Reactivity Trends Using the Concept of Group Softness. Journal of Physical Chemistry A, 2000, 104, 7639-7645.	2.5	49
20	Hierarchical Mesoporous RuO₂/Cu₂O Nanoparticle-Catalyzed Oxidative Homo/Hetero Azo-Coupling of Anilines. ACS Sustainable Chemistry and Engineering, 2018, 6, 11345-11352.	6.7	48
21	A variational method to calculate static electronic properties. Theoretica Chimica Acta, 1984, 66, 151-159.	0.8	46
22	Some aspects of self-consistent propagator theories. Physical Review A, 1985, 31, 1287-1298.	2.5	46
23	Analytically continued Fock space multireference coupled-cluster theory: Application to the Îg2 shape resonance in e-N2 scattering. Journal of Chemical Physics, 2005, 122, 234320.	3.0	42
24	Molecular recognition pattern of cytotoxic alkaloid vinblastine with multiple targets. Journal of Molecular Graphics and Modelling, 2014, 54, 1-9.	2.4	40
25	Nonlinear molecular properties using biorthogonal response approach. Journal of Chemical Physics, 1994, 101, 4914-4919.	3.0	37
26	Computational strategies for understanding the nature of interaction in dioxin imprinted nanoporous trappers. Journal of Molecular Recognition, 2015, 28, 427-437.	2.1	37
27	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
28	Metallo-Antiaromatic Al4Na4 and Al4Na3- Compounds:â€‰ A Theoretical Investigation. Journal of Physical Chemistry A, 2004, 108, 628-631.	2.5	36
29	N₂ activation on Al metal clusters: catalyzing role of BN-doped graphene support. Physical Chemistry Chemical Physics, 2016, 18, 27721-27727.	2.8	36
30	Use of a unitary wavefunction in the calculation of static electronic properties. Theoretica Chimica Acta, 1984, 66, 207-215.	0.8	35
31	Application of Hardâ^'Soft Acidâ^'Base Principle To Study BrÃ¶nsted Acid Sites in Zeolite Clusters:Â A Quantum Chemical Study. Journal of Physical Chemistry A, 1999, 103, 5978-5982.	2.5	35
32	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
33	Analysis of coupled-cluster methods for first-order static properties. Physical Review A, 1986, 33, 2240-2244.	2.5	34
34	Correlated complex independent particle potential for calculating electronic resonances. Journal of Chemical Physics, 2005, 123, 204110.	3.0	34
35	Effect of solvents having different dielectric constants on reactivity: A conceptual DFT approach. International Journal of Quantum Chemistry, 2010, 110, 1642-1647.	2.0	34
36	Fock space multi-reference coupled-cluster method for energies and energy derivatives. Molecular Physics, 2010, 108, 3033-3042.	1.7	34

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37	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
38	Development of a size-consistent energy functional for open shell states. Theoretica Chimica Acta, 1984, 66, 311-332.	0.8	32
39	Some novel relationships of polarizability with dipole moments. The Journal of Physical Chemistry, 1995, 99, 13865-13867.	2.9	32
40	A computational study of electronic structure, thermodynamics and kinetics of hydrogen desorption from Al- and Si-doped Î±-, Î³-, and Î²-MgH2. Journal of Materials Chemistry, 2009, 19, 4348.	6.7	32
41	Lithium bonding interaction in H2CYâ‹¯LiF (Y=O,S) complexes: A theoretical probe. Journal of Chemical Physics, 1997, 107, 4329-4336.	3.0	31
42	Minimum magnetizability principle. Journal of Chemical Physics, 2006, 125, 056101.	3.0	31
43	An open-shell coupled-cluster response method for static properties. International Journal of Quantum Chemistry, 1992, 41, 443-452.	2.0	30
44	Fock-space multireference coupled-cluster theory. fourth-order corrections to the ionization potential. Chemical Physics Letters, 1993, 209, 292-298.	2.6	30
45	Stationary coupled-cluster approaches to molecular properties: A comparative study. Physical Review A, 1996, 54, 250-258.	2.5	30
46	A constrained variational approach for energy derivatives in Fock-space multireference coupled-cluster theory. Journal of Chemical Physics, 2004, 120, 6381-6398.	3.0	30
47	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
48	Size- and Shape-Sensitive Reactivity Behavior of Al_n (n = 2â€“5, 13, 30, and 100) Clusters Toward the N₂ Molecule: A First-Principles Investigation. Journal of Physical Chemistry C, 2011, 115, 14615-14623.	3.1	30
49	CAP/EOM-CCSD method for the study of potential curves of resonant states. Physical Chemistry Chemical Physics, 2013, 15, 17915.	2.8	30
50	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
51	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
52	Energy Gap-Modulated Blue Phosphorene as Flexible Anodes for Lithium- and Sodium-Ion Batteries. Journal of Physical Chemistry C, 2019, 123, 2808-2819.	3.1	29
53	Development of an efficient linear response approach to the Hilbert space multi-reference coupled-cluster theory. Journal of Chemical Physics, 2001, 114, 1981-1988.	3.0	28
54	Density Functional Static Dipole Polarizability and First-Hyperpolarizability Calculations of Nan (n = 2,) Tj ETQq0 0 0 rgBT /Overlock 10 T Journal of Chemical Theory and Computation, 2007, 3, 716-727.	5.3	28

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55	Monolayer Transition-Metal Dichalcogenide Mo_{1â€“x}W_xS₂Alloys as Efficient Anode Materials for Lithium-Ion Batteries. Journal of Physical Chemistry C, 2018, 122, 25837-25848.	3.1	28
56	Bivariational coupled-cluster approach for the study of static electronicproperties/emph>. Physical Review A, 1986, 34, 2682-2686.	2.5	27
57	Intermediate Hamiltonian Hilbert space coupled cluster method: Theory and pilot application. International Journal of Quantum Chemistry, 2009, 109, 2909-2915.	2.0	27
58	Hydrogen Atom Chemisorbed Gold Clusters as Highly Active Catalysts for Oxygen Activation and CO Oxidation. Journal of Physical Chemistry C, 2014, 118, 30057-30062.	3.1	27
59	Relativistic equation-of-motion coupled-cluster method: Application to closed-shell atomic systems. Physical Review A, 2014, 89, .	2.5	27
60	Dipole moments of adiabatic excited states using the Fock space multireference coupled-cluster analytic response approach. Journal of Chemical Physics, 2001, 114, 3380-3384.	3.0	26
61	Ni(COD)₂-Catalyzed ipso-Silylation of 2-Methoxynaphthalene: A Density Functional Theory Study. Organometallics, 2018, 37, 1141-1149.	2.3	26
62	A general formalism of the Fock space multireference coupled cluster method for investigating molecular electronic resonances. Molecular Physics, 2005, 103, 2267-2275.	1.7	25
63	Dinitrogen Activation by Silicon and Phosphorus Doped Aluminum Clusters. Journal of Physical Chemistry C, 2014, 118, 19869-19878.	3.1	25
64	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
65	Implementation of a stationary coupled-cluster response method. Chemical Physics Letters, 1993, 211, 15-19.	2.6	24
66	Study of Local Hardâ^'Soft Acidâ^'Base Principle:Â Effects of Basis Set, Electron Correlation, and the Electron Partitioning Method. Journal of Physical Chemistry A, 2003, 107, 5755-5762.	2.5	24
67	Time-dependent multireference coupled-cluster-based response approach for evaluating dynamic properties. Physical Review A, 1997, 56, 2658-2664.	2.5	23
68	Dipole moments and polarizabilities of some small radicals using constrained variational response to Fock-space multi-reference coupled-cluster theory. Chemical Physics Letters, 2007, 438, 321-325.	2.6	23
69	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
70	Ab initio synthesis of linearly compensated zoom lenses by evolutionary programming. Applied Optics, 2011, 50, 1434.	2.1	20
71	Interatomic Coulombic decay in (n= 2â€“3) clusters using CAP/EOM-CCSD method. Molecular Physics, 2014, 112, 669-673.	1.7	20
72	Structure, energetics and bonding of diacetylene complexes with hydrogen fluoride. A theoretical investigation. Chemical Physics Letters, 1995, 247, 95-100.	2.6	19

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73	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
74	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
75	Search for parity and time reversal violating effects in HgH: Relativistic coupled-cluster study. Journal of Chemical Physics, 2016, 144, 124307.	3.0	19
76	Strain-engineered BluePâ€“MoS2 van der Waals heterostructure with improved lithiation/sodiation for LIBs and SIBs. Physical Chemistry Chemical Physics, 2020, 22, 1701-1714.	2.8	19
77	Adiabatic states of ozone using Fock space multireference coupled cluster method. Journal of Chemical Physics, 1999, 111, 4051-4055.	3.0	18
78	Density functional response approach for the linear and nonlinear electric properties of molecules. Journal of Chemical Physics, 2003, 118, 10861-10866.	3.0	18
79	Electric field response of molecular reactivity descriptors: a case study. Theoretical Chemistry Accounts, 2008, 120, 375-383.	1.4	18
80	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
81	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
82	Lower scaling approximation to EOMâ€CCSD: A critical assessment of the ionization problem. International Journal of Quantum Chemistry, 2018, 118, e25594.	2.0	18
83	Dipole moments of open-shell radicals using an analytic linear response approach in the Fock space multi-reference coupled cluster method. Chemical Physics Letters, 1999, 309, 457-462.	2.6	17
84	Calculation of Dipole Transition Matrix Elements and Expectation Values by Vibrational Coupled Cluster Method. Journal of Chemical Theory and Computation, 2010, 6, 3198-3204.	5.3	17
85	Molecular property calculations for excited states using a multireference coupled-cluster approach. Chemical Physics Letters, 1999, 300, 125-130.	2.6	16
86	Weak interaction between HCHY (Y=O, S) and LiCl: a theoretical study. Computational and Theoretical Chemistry, 2000, 497, 157-163.	1.5	16
87	Relativistic equation-of-motion coupled-cluster method for the double-ionization potentials of closed-shell atoms. Physical Review A, 2014, 90, .	2.5	16
88	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
89	Reactivity and Catalytic Activity of Hydrogen Atom Chemisorbed Silver Clusters. Journal of Physical Chemistry A, 2015, 119, 6162-6170.	2.5	16
90	Electron attachment to DNA and RNA nucleobases: An EOMCC investigation. International Journal of Quantum Chemistry, 2015, 115, 753-764.	2.0	16

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91	Endohedrally doped gold nanocages: efficient catalysts for O₂ activation and CO oxidation. Physical Chemistry Chemical Physics, 2016, 18, 7068-7074.	2.8	16
92	Coupled-cluster response approach: Improved variational strategy. Physical Review A, 1990, 42, 4385-4387.	2.5	15
93	Aberration correction of zoom lenses using evolutionary programming. Applied Optics, 2013, 52, 5724.	1.8	15
94	Study of approximate coupled cluster methods for first-order static properties. Theoretica Chimica Acta, 1985, 68, 379-388.	0.8	14
95	A Novel Theoretical Model for Molecular Recognition of Multiple-Site Interacting Systems Using Density Response Functions. Journal of Physical Chemistry B, 2001, 105, 4541-4544.	2.6	14
96	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
97	Bivariational coupled-cluster method: Equations for first-order property. Physical Review A, 1987, 36, 1539-1543.	2.5	13
98	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
99	Higher Energy Derivatives in Hilbert Space Multi-Reference Coupled Cluster Theory : A Constrained Variational Approach. International Journal of Molecular Sciences, 2002, 3, 710-732.	4.1	13
100	Molecular electric dipole moments using the GVVPT2 variant of multireference perturbation theory. Chemical Physics Letters, 2010, 487, 116-121.	2.6	13
101	Stabilization of pupils in a zoom lens with two independent movements. Applied Optics, 2013, 52, 5611.	1.8	13
102	Contriving a Catalytically Active Structure from an Inert Conformation: A Density Functional Investigation of Al, Hf, and Ge Doping of Au₂₀ Tetrahedral Clusters. Journal of Physical Chemistry C, 2016, 120, 19636-19641.	3.1	13
103	Multireference coupled cluster calculations on CH2+. Journal of Chemical Physics, 1992, 97, 3863-3864.	3.0	12
104	Z-vector formalism for the Fock space multireference coupled cluster method: Elimination of the response of the highest valence sector amplitudes. Journal of Chemical Physics, 1999, 111, 3832-3836.	3.0	12
105	Analytically continued Fock space multi-reference coupled-cluster theory: Application to the shape resonance. Chemical Physics, 2006, 329, 283-289.	1.9	12
106	Transition Metal Doped Aluminum Clusters: An Account of Spin. Journal of Physical Chemistry C, 2016, 120, 10027-10040.	3.1	11
107	Reactivity descriptors and electron density analysis for ligand chemistry: A case study of 2,2â€²-bipyridine and its analogues. Journal of Chemical Sciences, 2007, 119, 489-499.	1.5	10
108	Computational investigation on the catalytic activity of Rh6 and Rh4Ru2 clusters towards methanol activation. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	10

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109	Generalization of coupled-cluster response theory to multireference expansion spaces: application of the coupled-cluster singles and doubles effective Hamiltonian. Theoretical Chemistry Accounts, 1999, 102, 252-261.	1.4	9
110	A fully relaxed extended coupled-cluster approach for molecular properties. Chemical Physics Letters, 2004, 398, 194-200.	2.6	9
111	Analytical Dipole Moments and Dipole Polarizabilities of Oxygen Mono-Fluoride and Nitrogen Dioxide: A Constrained Variational Response to Fock-Space Multi-Reference Coupled-Cluster Method. Computing Letters, 2007, 3, 351-358.	0.5	9
112	Relativistic extended-coupled-cluster method for the magnetic hyperfine structure constant. Physical Review A, 2015, 91, .	2.5	9
113	Influence of carbon and phosphorus doping on electronic properties of ZnO. Journal of Materials Science: Materials in Electronics, 2016, 27, 12318-12322.	2.2	9
114	Dissociative Adsorption of Molecular Hydrogen on BN-Doped Graphene-Supported Aluminum Clusters. Journal of Physical Chemistry C, 2017, 121, 26493-26498.	3.1	9
115	Electronic structure parameter of nuclear magnetic quadrupole moment interaction in metal monofluorides. Journal of Chemical Physics, 2020, 153, 184306.	3.0	9
116	Analysis of coupled-cluster methods for higher-order static properties. Physical Review A, 1992, 45, 1518-1522.	2.5	8
117	Electric properties of BH, CO and H2O molecules by density functional response approach. Computational and Theoretical Chemistry, 2004, 676, 89-95.	1.5	8
118	Extended coupled cluster for Raman and infrared spectra of small molecules. Chemical Physics, 2012, 403, 25-32.	1.9	8
119	Role of substituents on the reactivity and electron density profile of diimine ligands: A density functional theory based study. Journal of Chemical Sciences, 2013, 125, 1247-1258.	1.5	8
120	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
121	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
122	2D Square Octagonal Molybdenum Disulfide: An Effective Anode Material for LIB/SIB Applications. Advanced Theory and Simulations, 2020, 3, 2000157.	2.8	8
123	Two-Dimensional Graphene/BlueP/MoS₂ van der Waals Multilayer Heterostructure as a High-Performance Anode Material for LIBs. Journal of Physical Chemistry C, 2021, 125, 8980-8992.	3.1	8
124	Studies on diacetylene complexes with water and ammonia. Chemical Physics Letters, 1995, 241, 399-403.	2.6	7
125	Structural design of mechanically compensated zoom lenses by evolutionary programming. Optical Engineering, 2012, 51, 063001.	1.0	7
126	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

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127	Correlation trends in the magnetic hyperfine structure of atoms: A relativistic coupled-cluster case study. Physical Review A, 2018, 98, .	2.5	7
128	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
129	Fock-Space Coupled Cluster Theory: Systematic Study of Partial Fourth Order Triples Schemes for Ionization Potential and Comparison with Bondonic Formalism. International Journal of Molecular Sciences, 2020, 21, 6199.	4.1	7
130	Atomistic details of effect of disulfide bond reduction on active site of Phytase B from Aspergillus niger: A MD Study. Bioinformation, 2013, 9, 963-967.	0.5	7
131	Unraveling the Effect of Aromatic Groups in Mn(I)NNN Pincer Complexes on Carbon Dioxide Activation Using Density Functional Study. Frontiers in Chemistry, 2021, 9, 778718.	3.6	7
132	Linearized bivariational coupled-cluster approach: General scheme for derivation of static properties. Physical Review A, 1989, 39, 2712-2714.	2.5	6
133	Polarizability of few electron quantum dots: Extended coupled-cluster response approach. Chemical Physics Letters, 2013, 555, 263-267.	2.6	6
134	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
135	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
136	Shape resonance of sulphur dioxide anion excited states using the CAP-CIP-FSMRCCSD method. Molecular Physics, 2020, 118, .	1.7	6
137	Separability of local reactivity descriptors. Journal of Chemical Sciences, 2005, 117, 497-505.	1.5	5
138	Constrained Variational Response to Fock-Space Multi-Reference Coupled-Cluster Theory: Formulation for Excited-State Electronic Structure Calculations and Some Pilot Applications. AIP Conference Proceedings, 2007, , .	0.4	5
139	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
140	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
141	Electron Detachment and Subsequent Structural Changes of Water Clusters. Journal of Physical Chemistry A, 2016, 120, 1065-1073.	2.5	5
142	Mechanistic Investigations of Aluminum Nitrite Assisted Aryl Nitrile Synthesis through C(sp³)â€“C(sp²) Bond Cleavage of Aryl Ketones. Journal of Physical Chemistry C, 2019, 123, 23439-23445.	3.1	5
143	Negative Ion Resonance States: The Fock-Space Coupled-Cluster Way. Journal of Physical Chemistry A, 2020, 124, 10407-10421.	2.5	5
144	Computational Exploration of the Efficacy of Fe(II)PNN Versus Fe(II)NNN Pincer Complexes in the Hydrogenation of Carbon Dioxide to Methanol. Journal of Physical Chemistry C, 2021, 125, 24350-24362.	3.1	5

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145	Haeckelite phosphorus: an emerging 2D allotrope of phosphorus for potential use in LIBs/SIBs. Physical Chemistry Chemical Physics, 2021, 23, 26547-26560.	2.8	5
146	An alternative definition of the electron propagator in the superoperator form and its relation to linear response theory in a coupled-cluster framework. Pramana - Journal of Physics, 1980, 15, 531-543.	1.8	4
147	Influence of bond length variation on correlated static exchange potential: A case study in eâ^'â€“N2 scattering. Journal of Chemical Physics, 1994, 100, 4712-4713.	3.0	4
148	Stationary multideterminantal coupled-cluster response. Physical Review A, 1994, 49, 1623-1628.	2.5	4
149	Understanding the molecular conformations of Na-dimyristoylphosphatidylglycerol (DMPG) using DFT-based method. Molecular Simulation, 2011, 37, 953-963.	2.0	4
150	NOx Catalyzed Pathway of Stratospheric Ozone Depletion: A Coupled Cluster Investigation. Journal of Chemical Theory and Computation, 2012, 8, 1895-1901.	5.3	4
151	Fock space multireference coupled cluster theory: Study of shape resonance. International Journal of Quantum Chemistry, 2013, 113, 1690-1695.	2.0	4
152	Understanding the orientation of water molecules around the phosphate and attached functional groups in a phospholipid molecule: a DFT-based study. Molecular Simulation, 2013, 39, 937-955.	2.0	4
153	Theoretical study of Câ€“X [XÂ=ÂCl, Br] bond activation on aluminum nanoclusters. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	4
154	Effect of Ligand Attachment on the Câ€“I Bond Dissociation Process on Aluminum Nanoclusters: A DFT Investigation. Journal of Physical Chemistry C, 2017, 121, 17354-17364.	3.1	4
155	Computational Approach to Unravel the Role of Hydrogen Bonding in the Interaction of NAMI-A with DNA Nucleobases and Nucleotides. Journal of Physical Chemistry A, 2018, 122, 8397-8411.	2.5	4
156	Applications of Multi-Reference Coupled-Cluster Theory. Lecture Notes in Quantum Chemistry II, 1989, , 143-153.	0.3	4
157	Stationary coupled cluster response: Role of cubic terms in molecular properties. Journal of Chemical Sciences, 1994, 106, 387-392.	1.5	4
158	Electron correlation effects in target molecule in low-energye? + N2 scattering. International Journal of Quantum Chemistry, 1995, 55, 291-297.	2.0	3
159	Study of constant term for electronâ€“molecule scattering: F2, H2CO and H2O target examples. Chemical Physics Letters, 2001, 345, 319-324.	2.6	3
160	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
161	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
162	Hydrogen bonding and non-covalent interaction assisted nickel(0) catalysed reversible alkenyl functional group swapping: a computational study. Catalysis Science and Technology, 2020, 10, 1747-1760.	4.1	3

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163	Three-Body Excitations in Fock-Space Coupled-Cluster: Fourth Order Perturbation Correction to Electron Affinity and Its Relation to Bondonic Formalism. International Journal of Molecular Sciences, 2021, 22, 8953.	4.1	3
164	On Some Aspects of Fock-Space Multi-Reference Coupled-Cluster Singles and Doubles Energies and Optical Properties. Challenges and Advances in Computational Chemistry and Physics, 2010, , 375-393.	0.6	3
165	Magnetizability of doublet radicals using Fock space multiâ€reference coupled cluster method. International Journal of Quantum Chemistry, 2009, 109, 2191-2198.	2.0	2
166	Behaviour of density functional theory for electric response properties at distorted geometries of molecules. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	2
167	Ground state of naphthyl cation: Singlet or triplet?. Journal of Chemical Physics, 2014, 140, 114312.	3.0	2
168	Calculation of hyperfine structure constants of small molecules using Z-vector method in the relativistic coupled-cluster framework. Journal of Chemical Sciences, 2016, 128, 1671-1675.	1.5	2
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