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	The Decisive Role of Spin States and Spin Coupling in Dictating Selective O ₂ Adsorption in Chromium(II) Metalâ€“Organic Frameworks. Chemistry - A European Journal, 2022, 28, e202200661.	3.3	1
2	Unraveling the Mechanistic Details of Ruâ€“Bis(pyridyl)borate Complex Catalyst for the Dehydrogenation of Ammonia Borane. Inorganic Chemistry, 2022, 61, 10283-10293.	4.0	2
3	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
4	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
5	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
6	Molecular frame dipole moment of diatomic molecules within relativistic <scp>coupledâ€cluster</scp> framework: A comparative study of expectation value versus energy derivative approach. International Journal of Quantum Chemistry, 2021, 121, e26764.	2.0	1
7	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
8	Partial fourth order schemes of triples in Fock-space coupled-cluster theory: Ionization potentials of ozone. Journal of the Indian Chemical Society, 2021, 98, 100166.	2.8	0
9	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
10	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
11	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
12	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
13	2D Square Octagonal Molybdenum Disulfide: An Effective Anode Material for LIB/SIB Applications. Advanced Theory and Simulations, 2020, 3, 2000157.	2.8	8
14	Negative Ion Resonance States: The Fock-Space Coupled-Cluster Way. Journal of Physical Chemistry A, 2020, 124, 10407-10421.	2.5	5
15	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
16	Electronic structure parameter of nuclear magnetic quadrupole moment interaction in metal monofluorides. Journal of Chemical Physics, 2020, 153, 184306.	3.0	9
17	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
18	Shape resonance of sulphur dioxide anion excited states using the CAP-CIP-FSMRCCSD method. Molecular Physics, 2020, 118, .	1.7	6

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19	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
20	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
21	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
22	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
23	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
24	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
25	Lower scaling approximation to EOMâ€CCSD: A critical assessment of the ionization problem. International Journal of Quantum Chemistry, 2018, 118, e25594.	2.0	18
26	Ni(COD)₂-Catalyzed ipso-Silylation of 2-Methoxynaphthalene: A Density Functional Theory Study. Organometallics, 2018, 37, 1141-1149.	2.3	26
27	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
28	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
29	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
30	Correlation trends in the magnetic hyperfine structure of atoms: A relativistic coupled-cluster case study. Physical Review A, 2018, 98, .	2.5	7
31	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
32	Dissociative Adsorption of Molecular Hydrogen on BN-Doped Graphene-Supported Aluminum Clusters. Journal of Physical Chemistry C, 2017, 121, 26493-26498.	3.1	9
33	Mechanistic Investigation of the Carbonâ€“Iodine Bond Activation on the Niobiumâ€“Carbon Cluster. ACS Omega, 2017, 2, 5335-5347.	3.5	2
34	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
35	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
36	Search for parity and time reversal violating effects in HgH: Relativistic coupled-cluster study. Journal of Chemical Physics, 2016, 144, 124307.	3.0	19

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37	Transition Metal Doped Aluminum Clusters: An Account of Spin. Journal of Physical Chemistry C, 2016, 120, 10027-10040.	3.1	11
38	Theoretical study of Câ€“X [XÂ=ÂCl, Br] bond activation on aluminum nanoclusters. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	4
39	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
40	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
41	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
42	N₂ activation on Al metal clusters: catalyzing role of BN-doped graphene support. Physical Chemistry Chemical Physics, 2016, 18, 27721-27727.	2.8	36
43	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
44	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
45	Endohedrally doped gold nanocages: efficient catalysts for O₂ activation and CO oxidation. Physical Chemistry Chemical Physics, 2016, 18, 7068-7074.	2.8	16
46	Electron Detachment and Subsequent Structural Changes of Water Clusters. Journal of Physical Chemistry A, 2016, 120, 1065-1073.	2.5	5
47	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
48	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
49	Reactivity and Catalytic Activity of Hydrogen Atom Chemisorbed Silver Clusters. Journal of Physical Chemistry A, 2015, 119, 6162-6170.	2.5	16
50	Computational strategies for understanding the nature of interaction in dioxin imprinted nanoporous trappers. Journal of Molecular Recognition, 2015, 28, 427-437.	2.1	37
51	Electron attachment to DNA and RNA nucleobases: An EOMCC investigation. International Journal of Quantum Chemistry, 2015, 115, 753-764.	2.0	16
52	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
53	Relativistic extended-coupled-cluster method for the magnetic hyperfine structure constant. Physical Review A, 2015, 91, .	2.5	9
54	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

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55	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
56	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
57	Computational investigation on the catalytic activity of Rh6 and Rh4Ru2 clusters towards methanol activation. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	10
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	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
60	Relativistic equation-of-motion coupled-cluster method: Application to closed-shell atomic systems. Physical Review A, 2014, 89, .	2.5	27
61	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
62	Ground state of naphthyl cation: Singlet or triplet?. Journal of Chemical Physics, 2014, 140, 114312.	3.0	2
63	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
64	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
65	Molecular recognition pattern of cytotoxic alkaloid vinblastine with multiple targets. Journal of Molecular Graphics and Modelling, 2014, 54, 1-9.	2.4	40
66	Interatomic Coulombic decay in (n= 2â€“3) clusters using CAP/EOM-CCSD method. Molecular Physics, 2014, 112, 669-673.	1.7	20
67	Dinitrogen Activation by Silicon and Phosphorus Doped Aluminum Clusters. Journal of Physical Chemistry C, 2014, 118, 19869-19878.	3.1	25
68	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
69	Relativistic equation-of-motion coupled-cluster method for the double-ionization potentials of closed-shell atoms. Physical Review A, 2014, 90, .	2.5	16
70	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
71	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
72	Fock space multireference coupled cluster theory: Study of shape resonance. International Journal of Quantum Chemistry, 2013, 113, 1690-1695.	2.0	4

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73	CAP/EOM-CCSD method for the study of potential curves of resonant states. Physical Chemistry Chemical Physics, 2013, 15, 17915.	2.8	30
74	Extended coupled cluster through nth perturbation order for molecular response properties: A comparative study. Chemical Physics, 2013, 417, 45-51.	1.9	0
75	Polarizability of few electron quantum dots: Extended coupled-cluster response approach. Chemical Physics Letters, 2013, 555, 263-267.	2.6	6
76	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
77	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
78	Stabilization of pupils in a zoom lens with two independent movements. Applied Optics, 2013, 52, 5611.	1.8	13
79	Aberration correction of zoom lenses using evolutionary programming. Applied Optics, 2013, 52, 5724.	1.8	15
80	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
81	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
82	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
83	Equation-of-motion coupled-cluster method for the study of shape resonance. Journal of Chemical Physics, 2012, 136, 234110.	3.0	54
84	Extended coupled cluster for Raman and infrared spectra of small molecules. Chemical Physics, 2012, 403, 25-32.	1.9	8
85	Structural design of mechanically compensated zoom lenses by evolutionary programming. Optical Engineering, 2012, 51, 063001.	1.0	7
86	NOx Catalyzed Pathway of Stratospheric Ozone Depletion: A Coupled Cluster Investigation. Journal of Chemical Theory and Computation, 2012, 8, 1895-1901.	5.3	4
87	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
88	Constrained variational approach for energy derivatives in Intermediate Hamiltonian Fock-space coupled-cluster theory. Chemical Physics, 2012, 401, 45-49.	1.9	1
89	Behaviour of density functional theory for electric response properties at distorted geometries of molecules. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	2
90	Descriptors as Probes for Inter-Molecular Interactions and External Perturbation. Structure and Bonding, 2012, , 131-158.	1.0	2

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91	Behaviour of density functional theory for electric response properties at distorted geometries of molecules. Highlights in Theoretical Chemistry, 2012, , 171-180.	0.0	0
92	Understanding the molecular conformations of Na-dimyristoylphosphatidylglycerol (DMPG) using DFT-based method. Molecular Simulation, 2011, 37, 953-963.	2.0	4
93	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
94	Ab initio synthesis of linearly compensated zoom lenses by evolutionary programming. Applied Optics, 2011, 50, 1434.	2.1	20
95	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
96	Molecular electric dipole moments using the GVVPT2 variant of multireference perturbation theory. Chemical Physics Letters, 2010, 487, 116-121.	2.6	13
97	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
98	Fock space multi-reference coupled-cluster method for energies and energy derivatives. Molecular Physics, 2010, 108, 3033-3042.	1.7	34
99	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
100	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
101	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
102	Magnetizability of doublet radicals using Fock space multiâ€reference coupled cluster method. International Journal of Quantum Chemistry, 2009, 109, 2191-2198.	2.0	2
103	Intermediate Hamiltonian Hilbert space coupled cluster method: Theory and pilot application. International Journal of Quantum Chemistry, 2009, 109, 2909-2915.	2.0	27
104	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
105	External Field Effects and Chemical Reactivity. , 2009, , .		2
106	Electric field response of molecular reactivity descriptors: a case study. Theoretical Chemistry Accounts, 2008, 120, 375-383.	1.4	18
107	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
108	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

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109	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
110	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
111	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
112	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
113	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
114	Analytically continued Fock space multi-reference coupled-cluster theory: Application to the shape resonance. Chemical Physics, 2006, 329, 283-289.	1.9	12
115	Minimum magnetizability principle. Journal of Chemical Physics, 2006, 125, 056101.	3.0	31
116	CALCULATION OF NEGATIVE ION SHAPE RESOANCES USING COUPLED CLUSTER THEORY. , 2006, , .		2
117	Separability of local reactivity descriptors. Journal of Chemical Sciences, 2005, 117, 497-505.	1.5	5
118	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
119	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
120	Correlated complex independent particle potential for calculating electronic resonances. Journal of Chemical Physics, 2005, 123, 204110.	3.0	34
121	Electric properties of molecules using stationary coupled-cluster method. Journal of Computational Methods in Sciences and Engineering, 2004, 4, 721-736.	0.2	0
122	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
123	Electric properties of BH, CO and H2O molecules by density functional response approach. Computational and Theoretical Chemistry, 2004, 676, 89-95.	1.5	8
124	A fully relaxed extended coupled-cluster approach for molecular properties. Chemical Physics Letters, 2004, 398, 194-200.	2.6	9
125	Aromaticity and antiaromaticity of LixAl4clusters: Ring current patterns versus electron counting. Physical Chemistry Chemical Physics, 2004, 6, 285-288.	2.8	76
126	Metallo-Antiaromatic Al4Na4 and Al4Na3- Compounds:â€‰ A Theoretical Investigation. Journal of Physical Chemistry A, 2004, 108, 628-631.	2.5	36

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127	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
128	Density functional response approach for the linear and nonlinear electric properties of molecules. Journal of Chemical Physics, 2003, 118, 10861-10866.	3.0	18
129	Study of Local Hardâ^'Soft Acidâ^'Base Principle to Multiple-Site Interactions. Journal of Physical Chemistry A, 2002, 106, 5737-5744.	2.5	52
130	Special Issue on Recent Advances in Coupled Cluster Theory. International Journal of Molecular Sciences, 2002, 3, 445-446.	4.1	0
131	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
132	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
133	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
134	Study of constant term for electronâ€"molecule scattering: F2, H2CO and H2O target examples. Chemical Physics Letters, 2001, 345, 319-324.	2.6	3
135	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
136	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
137	Weak interaction between HCHY (Y=O, S) and LiCl: a theoretical study. Computational and Theoretical Chemistry, 2000, 497, 157-163.	1.5	16
138	Intermolecular Reactivity Trends Using the Concept of Group Softness. Journal of Physical Chemistry A, 2000, 104, 7639-7645.	2.5	49
139	On non-negativity of Fukui function indices. II. Journal of Chemical Physics, 2000, 113, 1372-1379.	3.0	110
140	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
141	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
142	Adiabatic states of ozone using Fock space multireference coupled cluster method. Journal of Chemical Physics, 1999, 111, 4051-4055.	3.0	18
143	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
144	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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145	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
146	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
147	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
148	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
149	Fock space multireference coupled cluster theory: noniterative inclusion of triples for excitation energies. Theoretical Chemistry Accounts, 1998, 99, 100-105.	1.4	54
150	Time-dependent multireference coupled-cluster-based response approach for evaluating dynamic properties. Physical Review A, 1997, 56, 2658-2664.	2.5	23
151	ANALYTIC COUPLED CLUSTER BASED RESPONSE APPROACH USING MULTIDETERMINANTAL MODEL SPACE. Recent Advances in Computational, 1997, , 255-273.	0.8	0
152	Lithium bonding interaction in H2CYâ‹¯LiF (Y=O,S) complexes: A theoretical probe. Journal of Chemical Physics, 1997, 107, 4329-4336.	3.0	31
153	Stateâ€selective multireference coupledâ€cluster theory: In pursuit of property calculation. Journal of Chemical Physics, 1996, 104, 6582-6589.	3.0	56
154	Correlated staticâ€exchange interaction for electronâ€“molecule scattering: Case study for LiH and H2. Journal of Chemical Physics, 1996, 104, 9779-9782.	3.0	0
155	Stationary coupled-cluster approaches to molecular properties: A comparative study. Physical Review A, 1996, 54, 250-258.	2.5	30
156	Studies on diacetylene complexes with water and ammonia. Chemical Physics Letters, 1995, 241, 399-403.	2.6	7
157	Structure, energetics and bonding of diacetylene complexes with hydrogen fluoride. A theoretical investigation. Chemical Physics Letters, 1995, 247, 95-100.	2.6	19
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	Some novel relationships of polarizability with dipole moments. The Journal of Physical Chemistry, 1995, 99, 13865-13867.	2.9	32
160	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
161	Stationary multideterminantal coupled-cluster response. Physical Review A, 1994, 49, 1623-1628.	2.5	4
162	Nonlinear molecular properties using biorthogonal response approach. Journal of Chemical Physics, 1994, 101, 4914-4919.	3.0	37

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163	Stationary coupled cluster response: Role of cubic terms in molecular properties. Journal of Chemical Sciences, 1994, 106, 387-392.	1.5	4
164	Implementation of a stationary coupled-cluster response method. Chemical Physics Letters, 1993, 211, 15-19.	2.6	24
165	Fock-space multireference coupled-cluster theory. fourth-order corrections to the ionization potential. Chemical Physics Letters, 1993, 209, 292-298.	2.6	30
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