

Tapan K Ghanty

List of Publications by Year in descending order

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3,161
citations

159585

30
h-index

214800

47
g-index

138
all docs

138
docs citations

138
times ranked

2723
citing authors

#	ARTICLE	IF	CITATIONS
1	A Density Functional Approach to Hardness, Polarizability, and Valency of Molecules in Chemical Reactions. <i>The Journal of Physical Chemistry</i> , 1996, 100, 12295-12298.	2.9	180
2	Is the Hydrogen Bond in Water Dimer and Ice Covalent?. <i>Journal of the American Chemical Society</i> , 2000, 122, 1210-1214.	13.7	174
3	Ultrafast Intermolecular Hydrogen Bond Dynamics in the Excited State of Fluorenone. <i>Journal of Physical Chemistry A</i> , 2005, 109, 8693-8704.	2.5	100
4	Relationship between Ionization Potential, Polarizability, and Softness: A Case Study of Lithium and Sodium Metal Clusters. <i>Journal of Physical Chemistry A</i> , 2004, 108, 6661-6666.	2.5	92
5	Spin-Polarized Generalization of the Concepts of Electronegativity and Hardness and the Description of Chemical Binding. <i>Journal of the American Chemical Society</i> , 1994, 116, 3943-3948.	13.7	89
6	How strong is the interaction between a noble gas atom and a noble metal atom in the insertion compounds $MNgF$ ($M=Cu$ and Ag , and $Ng=Ar$, Kr , and Xe)?. <i>Journal of Chemical Physics</i> , 2006, 124, 124304.	3.0	77
7	Insertion of noble-gas atom (Kr and Xe) into noble-metal molecules (AuF and $AuOH$): Are they stable?. <i>Journal of Chemical Physics</i> , 2005, 123, 074323.	3.0	74
8	Structures and the Electronic Properties of Au_nX Clusters ($X = Li, Na, K, Rb, Cs, Cu$, and Tl)	3.1	68
9	Actinide selectivity of 1,10-phenanthroline-2,9-dicarboxamide and its derivatives: a theoretical prediction followed by experimental validation. <i>Dalton Transactions</i> , 2015, 44, 1332-1340.	3.3	60
10	Static dipole polarizability and binding energy of sodium clusters Na_n ($n=1-10$): A critical assessment of all-electron based post Hartree-Fock and density functional methods. <i>Journal of Chemical Physics</i> , 2004, 120, 6487-6494.	3.0	58
11	Complexation behavior of trivalent actinides and lanthanides with 1,10-phenanthroline-2,9-dicarboxylic acid based ligands: insight from density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 11060.	2.8	57
12	Hydrogen Bonding in Substituted Formic Acid Dimers. <i>Journal of Physical Chemistry A</i> , 2006, 110, 12623-12628.	2.5	48
13	Steric Strain Release-Directed Regioselective Functionalization of <i>meso</i> -Methyl Bodipy Dyes. <i>Organic Letters</i> , 2011, 13, 5870-5873.	4.6	45
14	Theoretical Prediction of Noble Gas Inserted Thioformyl Cations: $HNgCS^+$ ($Ng = He, Ne, Ar$)	2.9	45
15	Hardness and Polarizability Profiles for Intramolecular Proton Transfer in Water Dimer Radical Cation. <i>Journal of Physical Chemistry A</i> , 2002, 106, 4200-4204.	2.5	44
16	Electron Density and Energy Decomposition Analysis in Hydrogen-Bonded Complexes of Azabenzenes with Water, Acetamide, and Thioacetamide. <i>Journal of Physical Chemistry A</i> , 2005, 109, 7575-7582.	2.5	44
17	Polarizability of water clusters: An ab initio investigation. <i>Journal of Chemical Physics</i> , 2003, 118, 8547-8550.	3.0	42
18	Rational Design of Boradiazaindacene (BODIPY)-Based Functional Molecules. <i>Chemistry - A European Journal</i> , 2013, 19, 17766-17772.	3.3	41

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19	Electron spin resonance studies of $^{45}\text{Sc}^{17}\text{O}$, $^{89}\text{Y}^{17}\text{O}$, and $^{139}\text{La}^{17}\text{O}$ in rare gas matrices: Comparison with ab initio electronic structure and nuclear hyperfine calculations. <i>Journal of Chemical Physics</i> , 1999, 110, 5658-5669.	3.0	40
20	Diglycolamide-functionalized task specific ionic liquids for nuclear waste remediation: extraction, luminescence, theoretical and EPR investigations. <i>RSC Advances</i> , 2014, 4, 46613-46623.	3.6	40
21	Twisting Dynamics in the Excited Singlet State of Michler's Ketone. <i>Journal of Physical Chemistry A</i> , 2006, 110, 3432-3446.	2.5	38
22	Prediction of a New Series of Thermodynamically Stable Actinide Encapsulated Fullerene Systems Fulfilling the 32-Electron Principle. <i>Journal of Physical Chemistry C</i> , 2012, 116, 25630-25641.	3.1	37
23	Theoretical Prediction of Rare Gas Containing Hydride Cations: HRgBF_4^+ (Rg = He, Ar, Kr, Xe). <i>Journal of Physical Chemistry A</i> , 2007, 111, 7843-7852.	2.5	37
24	Theoretical Interpretation of the Photoelectron Spectra of Al_3O_2^- and Al_3O_3^- . <i>Journal of Physical Chemistry A</i> , 1999, 103, 8985-8993.	2.5	35
25	Ab Initio CASSCF and DFT Investigations of $(\text{H}_2\text{O})_2^+$ and $(\text{H}_2\text{S})_2^+$: Hemi-Bonded vs Proton-Transferred Structure. <i>Journal of Physical Chemistry A</i> , 2002, 106, 11815-11821.	2.5	34
26	Significant increase in the stability of rare gas hydrides on insertion of beryllium atom. <i>Journal of Chemical Physics</i> , 2007, 127, 114314.	3.0	34
27	Computational Modeling of Adsorption of Xe and Kr in M-MOF-74 Metal Organic Frame Works with Different Metal Atoms. <i>Journal of Physical Chemistry C</i> , 2016, 120, 10968-10974.	3.1	34
28	Electronegativity, hardness, and chemical binding in simple molecular systems. <i>Inorganic Chemistry</i> , 1992, 31, 1951-1955.	4.0	33
29	Heterocycle-Based Isomeric Chromophores with Substantially Varying NLO Properties: A New Structure-Property Correlation Study. <i>Journal of Physical Chemistry A</i> , 2008, 112, 4844-4852.	2.5	33
30	Theoretical Prediction of XRgCO^+ Ions (X = F, Cl, and Rg = Ar, Kr, Xe). <i>Journal of Physical Chemistry A</i> , 2013, 117, 14282-14292.	2.5	31
31	Theoretical investigation of electronic structure and ESR hyperfine parameters for the CuH^+ molecule. <i>International Journal of Quantum Chemistry</i> , 2000, 77, 291-300.	2.0	30
32	Reactions of Methyl Viologen Dication (MV_2^+) with H Atoms in Aqueous Solution: Mechanism Derived from Pulse Radiolysis Measurements and ab Initio MO Calculations. <i>Journal of Physical Chemistry A</i> , 2003, 107, 5998-6006.	2.5	30
33	Theoretical Prediction of Icosahedral U@C_{20} and Analogous Systems with High HOMO-LUMO Gap. <i>Journal of Physical Chemistry C</i> , 2012, 116, 16716-16725.	3.1	30
34	Diorgano-Gallium and -Indium Complexes Derived from Benzoazole Ligands: Synthesis, Characterization, Photoluminescence, and Computational Studies. <i>Organometallics</i> , 2013, 32, 104-111.	2.3	30
35	Structural and Chemical Properties of Subnanometer-Sized Bimetallic Au_{19}Pt Cluster. <i>Journal of Physical Chemistry C</i> , 2014, 118, 11935-11945.	3.1	30
36	Electronic Structure and Low-Lying Electronic States of Al_3O and Al_3O^- : Photoelectron Spectrum of Al_3O^- . <i>Journal of Physical Chemistry A</i> , 1999, 103, 2867-2872.	2.5	28

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37	Uncovering Heavy Actinide Covalency: Implications for Minor Actinide Partitioning. <i>Inorganic Chemistry</i> , 2019, 58, 3744-3753.	4.0	28
38	Molecular Hardness, Polarizability and Valency Variation of Formamide and Thioformamide on Internal Rotation: A Density Functional Study. <i>Journal of Physical Chemistry A</i> , 2000, 104, 2975-2979.	2.5	27
39	Complexation of trivalent lanthanides and actinides with several novel diglycolamide-functionalized calix[4]arenes: solvent extraction, luminescence and theoretical studies. <i>RSC Advances</i> , 2013, 3, 9296.	3.6	27
40	Highly selective separations of U(VI) from a Th(IV) matrix by branched butyl phosphates: Insights from solvent extraction, chromatography and quantum chemical calculations. <i>Separation and Purification Technology</i> , 2019, 210, 182-194.	7.9	27
41	Pu@C ₂₄ : A New Example Satisfying the 32-Electron Principle. <i>Journal of Physical Chemistry C</i> , 2014, 118, 7211-7221.	3.1	26
42	The Role of Hydrogen Bonding Interactions in the Ultrafast Relaxation Dynamics of the Excited States of 3-Amino- and 4-Amino-9-fluorenone. <i>ChemPhysChem</i> , 2009, 10, 2995-3012.	2.1	25
43	Synthesis, Characterization, Photoluminescence, and Computational Studies of Monoorgano-Gallium and -Indium Complexes Containing Dianionic Tridentate ONE (E = O or S) Schiff Bases. <i>Organometallics</i> , 2012, 31, 3836-3843.	2.3	25
44	Effect of Hydrogen Atom Doping on the Structure and Electronic Properties of 20-Atom Gold Cluster. <i>Journal of Physical Chemistry C</i> , 2016, 120, 18588-18594.	3.1	25
45	Adsorption and Activation of CO ₂ on Small-Sized Cu-Zr Bimetallic Clusters. <i>Journal of Physical Chemistry A</i> , 2021, 125, 2558-2572.	2.5	25
46	Nonlinear Optical Properties of Au ₁₉ M (M = Li, Na, K, Rb, Cs, Cu, Ag) Clusters. <i>Journal of Physical Chemistry C</i> , 2012, 116, 193-200.	3.1	24
47	Enhancement in the Stability of 36-Atom Fullerene through Encapsulation of a Uranium Atom. <i>Journal of Physical Chemistry C</i> , 2013, 117, 17859-17869.	3.1	24
48	Magic clusters MAu ₄ (M=Ti and Zr) and their dimers: How magic are they?. <i>Journal of Chemical Physics</i> , 2004, 120, 11363-11366.	3.0	23
49	Time-dependent density functional theory calculation of van der Waals coefficient of sodium clusters. <i>Journal of Chemical Physics</i> , 2007, 127, 134103.	3.0	23
50	Ab Initio Studies of Properties of Small Potassium Clusters. <i>Journal of Physical Chemistry A</i> , 2008, 112, 12303-12311.	2.5	23
51	Gold behaves as hydrogen: Prediction on the existence of a new class of boron-containing radicals, AuBX (X=F,Cl,Br). <i>Journal of Chemical Physics</i> , 2005, 123, 241101.	3.0	22
52	Structural Investigation of Asymmetrical Dimer Radical Cation System (H ₂ O...H ₂ S) ⁺ : Proton-Transferred or Hemi-Bonded?. <i>Journal of Physical Chemistry A</i> , 2007, 111, 2362-2367.	2.5	22
53	Significant modulation of CO adsorption on bimetallic Au ₁₉ Li cluster. <i>Chemical Physics</i> , 2014, 428, 75-81.	1.9	22
54	Noble-Gas-Inserted Fluoro(sulphido)boron (FN _g BS, N _g = Ar, Kr, and Xe): A Theoretical Prediction. <i>Journal of Physical Chemistry A</i> , 2015, 119, 5732-5741.	2.5	22

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55	Ab initio studies on the polarizability of lithium clusters: Some unusual results. International Journal of Quantum Chemistry, 2005, 105, 166-173.	2.0	21
56	A sum-over-state scheme of analysis of hyperpolarizabilities and its application to spiroconjugated molecular system. Theoretical Chemistry Accounts, 2010, 126, 323-337.	1.4	21
57	Polarizability, Ionization Potential, and Softness of Water and Methanol Clusters: An Interrelation. Journal of Physical Chemistry A, 2012, 116, 6831-6836.	2.5	21
58	Theoretical prediction of rare gas inserted hydronium ions: HRgOH ₂ ⁺ . Journal of Chemical Physics, 2013, 138, 194308.	3.0	21
59	Prediction of neutral noble gas insertion compounds with heavier pnictides: FNgY (Ng = Kr and Xe; Y =) Tj ETQq1 1 0,784314,rgBT /Over 2.8 2F	2.8	21
60	Hydrogen-Bonding Interactions in Selected Super-molecular Systems: Electron Density Point of View. Journal of Physical Chemistry A, 2003, 107, 7062-7067.	2.5	20
61	Theoretical Study of the Effect of Structural Modifications on the Hyperpolarizabilities of Indigo Derivatives. Journal of Physical Chemistry A, 2009, 113, 2623-2631.	2.5	19
62	Confinement-Directed Adsorption of Noble Gases (Xe/Kr) in MFM-300(M)-Based Metal-Organic Framework Materials. Journal of Physical Chemistry C, 2019, 123, 27531-27541.	3.1	19
63	A peculiar excited electronic state of allene (1,2-propadiene). Chemical Physics Letters, 1998, 287, 61-69.	2.6	18
64	Unprecedented Enhancement of Noble Gas Noble Metal Bonding in NgAu ₃ ⁺ (Ng = Ar, Kr, and Xe) Ion through Hydrogen Doping. Journal of Physical Chemistry A, 2016, 120, 9998-10006.	2.5	18
65	Hydrogen Bonding in Neutral and Cation Dimers of H ₂ Se with H ₂ O, H ₂ S, and H ₂ Se. Journal of Physical Chemistry A, 2012, 116, 11965-11972.	2.5	17
66	Density functional investigation on the structures and properties of Li atom doped Au ₂₀ cluster. Molecular Physics, 2013, 111, 725-734.	1.7	16
67	Structure and Stability of Zn, Cd, and Hg Atom Doped Golden Fullerene (Au ₃₂). Journal of Physical Chemistry C, 2013, 117, 18777-18788.	3.1	16
68	Prediction of a Neutral Noble Gas Compound in the Triplet State. Chemistry - A European Journal, 2015, 21, 8290-8296.	3.3	16
69	Noble Gas Encapsulated Endohedral Zintl Ions Ng@Pb ₁₂ ²⁺ and Ng@Sn ₁₂ ²⁺ (Ng = He, Ne, Ar, and Kr): A Theoretical Investigation. Journal of Physical Chemistry C, 2017, 121, 11932-11949.	3.1	16
70	Experimental evidence and quantum chemical insights into extraction and third phase aggregation trends in Ce(IV) organophosphates. Separation and Purification Technology, 2019, 217, 62-70.	7.9	16
71	Proton Affinity and Acidity of Hypohalous Acids: A Density Functional Study. Journal of Physical Chemistry A, 1997, 101, 5022-5025.	2.5	15
72	Electronic structure and thermophysical properties of U ₃ Si ₂ : A systematic first principle study. Journal of Nuclear Materials, 2018, 510, 360-365.	2.7	15

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73	Quantum chemical prediction of a superelectrophilic dianion and its binding with noble gas atoms. <i>Chemical Communications</i> , 2019, 55, 14379-14382.	4.1	15
74	Excited state polarizabilities of methanol clusters. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 2929.	2.8	14
75	Noble Gas Inserted Protonated Silicon Monoxide Cations: $\text{HNgOSi}^+ (\text{Ng} = \text{He, Ne, Ar, Kr})$. <i>Journal of Physical Chemistry A</i> , 2019, 123, 10784-10794.	2.5	14
76	Adsorption properties of fission gases Xe and Kr on pristine and doped graphene: A first principle DFT study. <i>Journal of Nuclear Materials</i> , 2017, 490, 174-180.	2.7	14
77	Study of Adsorption of Fission Gas Atoms Xe and Kr on MoS_2 Monolayer Functionalized with 3d Transition Metals. <i>Journal of Physical Chemistry C</i> , 2021, 125, 1493-1508.	3.1	14
78	Ionized State of Hydroperoxy Radical \cdot Water Hydrogen-Bonded Complex: $(\text{HO}_2\cdot\text{H}_2\text{O})^+$. <i>Journal of Physical Chemistry A</i> , 2007, 111, 13590-13594.	2.5	13
79	Synthesis, characterization, photoluminescence and computational studies of mono- and diorgano-gallium complexes containing azo linked salicylaldehyde Schiff bases. <i>Journal of Organometallic Chemistry</i> , 2015, 776, 98-106.	1.8	13
80	Theoretical prediction of noble gas inserted halocarbenes: FNgcX ($\text{Ng} = \text{Kr, and Xe; X} = \text{F, Cl, Br, and I}$). <i>Chemical Physics</i> , 2017, 494, 20-30.	1.9	13
81	A new electronegativity based approach to the calculation of partial atomic charges and other related reactivity indices in molecules. <i>Computational and Theoretical Chemistry</i> , 1992, 276, 83-96.	1.5	12
82	Formation of semiquinone radical in the reaction of embelin (2,5-dihydroxy-3-undecyl-1,4-benzoquinone) with reductants as well as oxidants. Characterization by pulse radiolysis and structure investigation by quantum chemical study. <i>Journal of Molecular Structure</i> , 2009, 928, 46-53.	3.6	12
83	Structure and solvent-induced tuning of laser property and photostability of a boradiazaindacene (BODIPY) dye. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2017, 349, 162-170.	3.9	12
84	Remarkable structural effects on the complexation of actinides with H-phosphonates: a combined experimental and quantum chemical study. <i>Dalton Transactions</i> , 2018, 47, 3841-3850.	3.3	12
85	Unprecedented stability enhancement of multiply charged anions through decoration with negative electron affinity noble gases. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 13368-13372.	2.8	12
86	Fluorescent Cu^{2+} sensor based on phenanthroline-BODIPY conjugate: A mechanistic study. <i>Dyes and Pigments</i> , 2022, 203, 110343.	3.7	12
87	Noble gas hydrides in the triplet state: $\text{HNgcCO}^+ (\text{Ng} = \text{He, Ne, Ar, Kr, and Xe})$. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 20270-20279.	2.8	11
88	Adsorption and activation of CO_2 on Zr_n ($n = 2-7$) clusters. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 16877-16886.	2.8	11
89	Hydration of uranyl cations: Effective fragment potential approach. <i>Computational and Theoretical Chemistry</i> , 2007, 807, 93-99.	1.5	10
90	Interesting periodic variations in physical and chemical properties of homonuclear diatomic molecules. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 1097-1106.	2.0	10

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91	Does enhanced oxygen activation always facilitate CO oxidation on gold clusters?. <i>Journal of Computational Chemistry</i> , 2015, 36, 2177-2187.	3.3	10
92	An Insight into the Complexation of Trivalent Americium with Bis(1,2,4-triazinyl)bipyridine Derivatives. <i>European Journal of Inorganic Chemistry</i> , 2017, 2017, 820-828.	2.0	10
93	Role of metcar on the adsorption and activation of carbon dioxide: a DFT study. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 5559-5570.	2.8	10
94	A new simple approach to the polarizability of atoms and ions using frontier orbitals from the Kohn-Sham density functional theory. <i>Computational and Theoretical Chemistry</i> , 1996, 366, 139-144.	1.5	9
95	Silicene: A Promising Surface to Achieve Morphological Transformation in Gold Clusters. <i>Journal of Physical Chemistry C</i> , 2015, 119, 3192-3198.	3.1	9
96	Substituent effect on ionization potential, O-H bond dissociation energy and intra-molecular hydrogen bonding in salicylic acid derivatives. <i>Computational and Theoretical Chemistry</i> , 2010, 948, 47-54.	1.5	8
97	Hydrogen-bonded complexes of nicotine with simple alcohols. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 2787-2793.	2.0	8
98	Theoretical investigation of M@Pb_{12}^{2+} and M@Sn_{12}^{2+} Zintl clusters (M = Lr_{n+} , Lu_{n+}), <i>Journal of Physical Chemistry C</i> , 2019, 123, 15253-15272.	2.8	8
99	Remarkable Structural Effect on the Gold-Hydrogen Analogy in Hydrogen-Doped Gold Cluster. <i>Journal of Physical Chemistry A</i> , 2019, 123, 1973-1982.	2.5	8
100	Reactions and structural investigation of chlorpromazine radical cation. <i>Journal of Molecular Structure</i> , 2008, 888, 401-408.	3.6	7
101	Atom- and Ion-Centered Icosahedral Shaped Subnanometer-Sized Clusters of Molecular Hydrogen. <i>Journal of Physical Chemistry C</i> , 2017, 121, 15036-15048.	3.1	7
102	Hybrid Organic-Inorganic Functionalized Dodecaboranes and Their Potential Role in Lithium and Magnesium Ion Batteries. <i>Journal of Physical Chemistry C</i> , 2018, 122, 27947-27954.	3.1	7
103	Structure-Modulated Complexation of Actinides with Phosphonates: A Combined Experimental and Quantum Chemical Investigation. <i>ChemistrySelect</i> , 2018, 3, 11309-11315.	1.5	7
104	On the position of La, Lu, Ac and Lr in the periodic table: a perspective. <i>Journal of Chemical Sciences</i> , 2019, 131, 1.	1.5	7
105	The effect of doping on adsorption of Xe and Kr on graphyne and graphdiyne. <i>Materials Today Communications</i> , 2020, 22, 100738.	1.9	7
106	Dopant-Free, Blue-Light-Emitting, Hydrophobic Deep Eutectic Solvent and Its Application as a Liquid Scintillator. <i>ACS Applied Electronic Materials</i> , 2022, 4, 2175-2179.	4.3	7
107	Density functional study of the relationship between energy, hardness, and polarizability of molecules in nonequilibrium situations. <i>International Journal of Quantum Chemistry</i> , 1997, 63, 917-926.	2.0	6
108	Predicted $\text{M}(\text{H}_2)_{12n+}$ (M = Ac, Th, Pa, U, La and n = 3, 4) complexes with twenty-four hydrogen atoms bound to the metal ion. <i>Chemical Communications</i> , 2019, 55, 7788-7791.	4.1	6

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109	Strong influence of weak hydrogen bonding on actinide ²⁺ phosphonate complexation: accurate predictions from DFT followed by experimental validation. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 5566-5577.	2.8	6
110	Anomaly in the stability of the hydroxides of icosagens (B and Al) and their noble gas (Xe and Rn) derivatives: a comparative study. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 14109-14124.	2.8	6
111	Time-dependent density functional theory calculation of van der Waals coefficient of potassium clusters. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 1376-1384.	2.0	5
112	Hydrogen bonding interaction between HO ₂ radical and selected organic acids, RCOOH (R=CH ₃ , H, Cl) <i>Tj ETQq0 0,0 rgBT /Ovlock 10</i>	2.6	5
113	Synthesis and Characterization of Some BODIPY-based Substituted Salicylaldehyde Schiff Bases. <i>Journal of Heterocyclic Chemistry</i> , 2019, 56, 2499-2507.	2.6	5
114	Lanthanide and actinide doped B ₁₂ H ₁₂ ²⁺ and Al ₁₂ H ₁₂ ²⁺ clusters: new magnetic superatoms with f-block elements. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 23720-23732.	2.8	5
115	Adsorption control of Xe and Kr in SBMOF-2 metal-organic framework by ligand functionalization and different metal atoms. <i>Computational Materials Science</i> , 2021, 189, 110264.	3.0	5
116	Exploration of N-oxo pyridine 2-carboxamide ligands towards coordination chemistry, solvent extraction, and DFT investigation for the development of novel solvent for lanthanide and actinide separation. <i>Polyhedron</i> , 2021, 201, 115166.	2.2	5
117	Strain Engineering of 2D-C ₃ N ₅ Monolayer and Its Application in Overall Water-Splitting: a Hybrid Density Functional Study. <i>Journal of Physical Chemistry C</i> , 2022, 126, 8436-8449.	3.1	5
118	Structure of thiocyanate dimer radical anion: An ab initio study. <i>Computational and Theoretical Chemistry</i> , 2005, 723, 235-239.	1.5	4
119	Theoretical prediction of FN ₃ M ₃ (N = Ar, Kr, Xe, and Rn; M = Cu, Ag and Au; Q = 0, +2) molecules <i>Molecular Physics</i> , 0, , .	1.7	4
120	Stability-Order Reversal in FS _Y and FY _{Si} (Y = N and P) Molecules after the Insertion of a Noble Gas Atom. <i>Journal of Physical Chemistry A</i> , 2022, 126, 1132-1143.	2.5	4
121	Reassignment of the AlSi photoelectron spectrum by ab initio configuration interaction calculations. <i>Molecular Physics</i> , 1999, 96, 735-740.	1.7	3
122	Hydrogen bonding interaction in complexes of hydronium ion with selective chemical species. <i>Chemical Physics Letters</i> , 2009, 471, 36-40.	2.6	3
123	Structural diversity ranging from cyclic trimeric, tetrameric, hexameric to 1-D helix in dimethylgallium hydroxide. <i>Journal of Organometallic Chemistry</i> , 2015, 781, 65-71.	1.8	3
124	Exploring the electronic structure and thermal properties of UAl ₃ using density functional theory calculations. <i>Journal of Physics and Chemistry of Solids</i> , 2020, 136, 109179.	4.0	3
125	Reassignment of the AlSi photoelectron spectrum by ab initio configuration interaction calculations. <i>Molecular Physics</i> , 1999, 96, 735-740.	1.7	3
126	Ab initio calculations on XF _n Q (X = I, Xe, Cs, and Ba; n=1, 2, 4, and 6; q=?1, 0, +1, and +2) molecules. <i>International Journal of Quantum Chemistry</i> , 2001, 81, 238-245.	2.0	2

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127	Prediction of a Nine-Membered Aromatic Heterocyclic 1,4,7-triazacyclononatetraenyl anion and its Sandwich Complexes with Divalent Lanthanides. <i>ChemistrySelect</i> , 2019, 4, 9940-9946.	1.5	2
128	A combined experimental and quantum chemical studies on the structure and binding preferences of picolinamide based ligands with uranyl nitrate. <i>Polyhedron</i> , 2019, 171, 486-492.	2.2	2
129	Adsorption and activation of CO ₂ molecule on subnanometer-sized anionic vanadium carbide clusters V _n C _{4-n} (n = 1-6): A theoretical study. <i>Molecular Catalysis</i> , 2021, 515, 111871.	2.0	2
130	Electronegativity-based approach to a new potential energy function for bond extensions. <i>Computational and Theoretical Chemistry</i> , 1994, 309, 143-149.	1.5	1
131	Structure and binding energies of halogenated hydroxymethoxy radical-water hydrogen-bonded complexes: HOC(X)(Y)O·-nH ₂ O (n=0, 1, 2 and X, Y=H/F/Cl). <i>Computational and Theoretical Chemistry</i> , 2012, 992, 30-36.	2.5	1
132	A first-principles study of the effect of oxygen vacancy on rutile Ti _{1-x} CdxO ₂ . <i>Solid State Communications</i> , 2012, 152, 142-146.	1.9	1
133	Synthesis, Characterization, Photophysical and DFT Studies of Coumarin Schiff Bases and Their Dimethylgallium Complexes. <i>Proceedings of the National Academy of Sciences India Section A - Physical Sciences</i> , 2016, 86, 633-644.	1.2	1
134	Counter-Intuitive Stability in Actinide-Encapsulated Metalloid Clusters with Broken Aromaticity. <i>Journal of Physical Chemistry C</i> , 2018, 122, 22469-22479.	3.1	1
135	The Decisive Role of Spin States and Spin Coupling in Dictating Selective O ₂ Adsorption in Chromium(II) Metal-Organic Frameworks. <i>Chemistry - A European Journal</i> , 2022, 28, e202200661.	3.3	1
136	THEORETICAL STUDIES ON POLARIZABILITY OF ALKALI METAL CLUSTERS. , 2006, , 625-655.		0
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