Tapan K Ghanty

List of Publications by Year
in descending order

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137 papers	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	Stability-Order Reversal in FSiY and FYSi (Y = N and P) Molecules after the Insertion of a Noble Gas Atom. Journal of Physical Chemistry A, 2022, 126, 1132-1143.	2.5	4
2	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
3	Dopant-Free, Blue-Light-Emitting, Hydrophobic Deep Eutectic Solvent and Its Application as a Liquid Scintillator. ACS Applied Electronic Materials, 2022, 4, 2175-2179.	4.3	7
4	Strain Engineering of 2D-C₃N₅ Monolayer and Its Application in Overall Water-Splitting: a Hybrid Density Functional Study. Journal of Physical Chemistry C, 2022, 126, 8436-8449.	3.1	5
5	Fluorescent Cu2+ sensor based on phenanthroline-BODIPY conjugate: A mechanistic study. Dyes and Pigments, 2022, 203, 110343.	3.7	12
6	Role of metcar on the adsorption and activation of carbon dioxide: a DFT study. Physical Chemistry Chemical Physics, 2021, 23, 5559-5570.	2.8	10
7	Ab Initio Study of Adsorption of Fission Gas Atoms Xe and Kr on MoS₂ Monolayer Functionalized with 3d Transition Metals. Journal of Physical Chemistry C, 2021, 125, 1493-1508.	3.1	14
8	Adsorption and Activation of CO₂ on Small-Sized Cuâ€“Zr Bimetallic Clusters. Journal of Physical Chemistry A, 2021, 125, 2558-2572.	2.5	25
9	Adsorption control of Xe and Kr in SBMOF-2 metal-organic framework by ligand functionalization and different metal atoms. Computational Materials Science, 2021, 189, 110264.	3.0	5
10	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. Polyhedron, 2021, 201, 115166.	2.2	5
11	Adsorption and activation of CO2 molecule on subnanometer-sized anionic vanadium carbide clusters V C4â¯ (n = 1â€“6): A theoretical study. Molecular Catalysis, 2021, 515, 111871.	2.0	2
12	Exploring the electronic structure and thermal properties of UAl3 using density functional theory calculations. Journal of Physics and Chemistry of Solids, 2020, 136, 109179.	4.0	3
13	The effect of doping on adsorption of Xe and Kr on graphyne and graphdiyne. Materials Today Communications, 2020, 22, 100738.	1.9	7
14	Unprecedented stability enhancement of multiply charged anions through decoration with negative electron affinity noble gases. Physical Chemistry Chemical Physics, 2020, 22, 13368-13372.	2.8	12
15	Adsorption and activation of CO₂ on Zr_n (n = 2â€“7) clusters. Physical Chemistry Chemical Physics, 2020, 22, 16877-16886.	2.8	11
16	Anomaly in the stability of the hydroxides of icosagens (B and Al) and their noble gas (Xe and Rn) derivatives: a comparative study. Physical Chemistry Chemical Physics, 2020, 22, 14109-14124.	2.8	6
17	Highly selective separations of U(VI) from a Th(IV) matrix by branched butyl phosphates: Insights from solvent extraction, chromatography and quantum chemical calculations. Separation and Purification Technology, 2019, 210, 182-194.	7.9	27
18	Synthesis and Characterization of Some BODIPYâ€based Substituted Salicylaldimine Schiff Bases. Journal of Heterocyclic Chemistry, 2019, 56, 2499-2507.	2.6	5

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19	Prediction of a Nineâ^'Membered Aromatic Heterocyclic 1,4,7â^'triazacyclononatetraenyl anion and its Sandwich Complexes with Divalent Lanthanides. ChemistrySelect, 2019, 4, 9940-9946.	1.5	2
20	Confinement-Directed Adsorption of Noble Gases (Xe/Kr) in MFM-300(M)-Based Metalâ€"Organic Framework Materials. Journal of Physical Chemistry C, 2019, 123, 27531-27541.	3.1	19
21	A combined experimental and quantum chemical studies on the structure and binding preferences of picolinamide based ligands with uranyl nitrate. Polyhedron, 2019, 171, 486-492.	2.2	2
22	Predicted M(H2)12n+ (M = Ac, Th, Pa, U, La and n = 3, 4) complexes with twenty-four hydrogen atoms bound to the metal ion. Chemical Communications, 2019, 55, 7788-7791.	4.1	6
23	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
24	Remarkable Structural Effect on the Goldâ€"Hydrogen Analogy in Hydrogen-Doped Gold Cluster. Journal of Physical Chemistry A, 2019, 123, 1973-1982.	2.5	8
25	Uncovering Heavy Actinide Covalency: Implications for Minor Actinide Partitioning. Inorganic Chemistry, 2019, 58, 3744-3753.	4.0	28
26	Strong influence of weak hydrogen bonding on actinideâ€"phosphonate complexation: accurate predictions from DFT followed by experimental validation. Physical Chemistry Chemical Physics, 2019, 21, 5566-5577.	2.8	6
27	Quantum chemical prediction of a superelectrophilic dianion and its binding with noble gas atoms. Chemical Communications, 2019, 55, 14379-14382.	4.1	15
28	Lanthanide and actinide doped B12H122â^' and Al12H122â^' clusters: new magnetic superatoms with f-block elements. Physical Chemistry Chemical Physics, 2019, 21, 23720-23732.	2.8	5
29	On the position of La, Lu, Ac and Lr in the periodic table: a perspective. Journal of Chemical Sciences, 2019, 131, 1.	1.5	7
30	Remarkable structural effects on the complexation of actinides with H-phosphonates: a combined experimental and quantum chemical study. Dalton Transactions, 2018, 47, 3841-3850.	3.3	12
31	Theoretical investigation of M@Pb₁₂^{2â^'} and M@Sn₁₂^{2â^'} Zintl clusters (M = Lrⁿ⁺, Luⁿ⁺,) Tj ETQq1 1 0.784314 rgBT /Overloc 20, 15253-15272.	2.8	8
32	Hybrid Organicâ€"Inorganic Functionalized Dodecaboranes and Their Potential Role in Lithium and Magnesium Ion Batteries. Journal of Physical Chemistry C, 2018, 122, 27947-27954.	3.1	7
33	Structureâ€Modulated Complexation of Actinides with Phosphonates: A Combined Experimental and Quantum Chemical Investigation. ChemistrySelect, 2018, 3, 11309-11315.	1.5	7
34	Counter-Intuitive Stability in Actinide-Encapsulated Metalloid Clusters with Broken Aromaticity. Journal of Physical Chemistry C, 2018, 122, 22469-22479.	3.1	1
35	Noble gas hydrides in the triplet state: HNgCCO⁺ (Ng = He, Ne, Ar, Kr, and Xe). Physical Chemistry Chemical Physics, 2018, 20, 20270-20279.	2.8	11
36	Electronic structure and thermophysical properties of U3Si2: A systematic first principle study. Journal of Nuclear Materials, 2018, 510, 360-365.	2.7	15

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37	Adsorption properties of fission gases Xe and Kr on pristine and doped graphene: A first principle DFT study. Journal of Nuclear Materials, 2017, 490, 174-180.	2.7	14
38	Noble Gas Encapsulated Endohedral Zintl Ions Ng@Pb₁₂^{2â€“} and Ng@Sn₁₂^{2â€“} (Ng = He, Ne, Ar, and Kr): A Theoretical Investigation. Journal of Physical Chemistry C, 2017, 121, 11932-11949.	3.1	16
39	Atom- and Ion-Centered Icosahedral Shaped Subnanometer-Sized Clusters of Molecular Hydrogen. Journal of Physical Chemistry C, 2017, 121, 15036-15048.	3.1	7
40	Structure and solvent-induced tuning of laser property and photostability of a boradiazaindacene (BODIPY) dye. Journal of Photochemistry and Photobiology A: Chemistry, 2017, 349, 162-170.	3.9	12
41	Theoretical prediction of noble gas inserted halocarbenes: FNgCX (Ng = Kr, and Xe; X = F, Cl, Br, and I). Chemical Physics, 2017, 494, 20-30.	1.9	13
42	An Insight into the Complexation of Trivalent Americium Visâ€Ââ€Vis Lanthanides with Bis(1,2,4â€triazinyl)bipyridine Derivatives. European Journal of Inorganic Chemistry, 2017, 2017, 820-828.	2.0	10
43	Prediction of neutral noble gas insertion compounds with heavier pnictides: FNgY (Ng = Kr and Xe; Y =) Tj ETQq1 1 0.784314 rgBT /Ov	2.8	21
44	Computational Modeling of Adsorption of Xe and Kr in M-MOF-74 Metal Organic Frame Works with Different Metal Atoms. Journal of Physical Chemistry C, 2016, 120, 10968-10974.	3.1	34
45	Synthesis, Characterization, Photophysical and DFT Studies of Coumarin Schiff Bases and Their Dimethylgallium Complexes. Proceedings of the National Academy of Sciences India Section A - Physical Sciences, 2016, 86, 633-644.	1.2	1
46	Effect of Hydrogen Atom Doping on the Structure and Electronic Properties of 20-Atom Gold Cluster. Journal of Physical Chemistry C, 2016, 120, 18588-18594.	3.1	25
47	Unprecedented Enhancement of Noble Gasâ€“Noble Metal Bonding in NgAu₃⁺ (Ng = Ar, Kr, and Xe) Ion through Hydrogen Doping. Journal of Physical Chemistry A, 2016, 120, 9998-10006.	2.5	18
48	Does enhanced oxygen activation always facilitate <scp>CO</scp> oxidation on gold clusters?. Journal of Computational Chemistry, 2015, 36, 2177-2187.	3.3	10
49	Prediction of a Neutral Noble Gas Compound in the Triplet State. Chemistry - A European Journal, 2015, 21, 8290-8296.	3.3	16
50	Noble Gas Inserted Protonated Silicon Monoxide Cations: HNgOSi⁺ (Ng = He, Ne, Ar, Kr,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	2.5	14
51	Structural diversity ranging from cyclic trimeric, tetrameric, hexameric to 1-D helix in dimethylgallium hydroxide. Journal of Organometallic Chemistry, 2015, 781, 65-71.	1.8	3
52	Silicene: A Promising Surface to Achieve Morphological Transformation in Gold Clusters. Journal of Physical Chemistry C, 2015, 119, 3192-3198.	3.1	9
53	Noble-Gas-Inserted Fluoro(sulphido)boron (FNgBS, Ng = Ar, Kr, and Xe): A Theoretical Prediction. Journal of Physical Chemistry A, 2015, 119, 5732-5741.	2.5	22
54	Synthesis, characterization, photoluminescence and computational studies of mono- and diorgano-gallium complexes containing azo linked salicylaldimine Schiff bases. Journal of Organometallic Chemistry, 2015, 776, 98-106.	1.8	13

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55	Theoretical Prediction of Noble Gas Inserted Thioformyl Cations: HNgCS⁺ (Ng = He, Ne, Ar,) Tj ETQq1 1 0.784314 rgBT /O	2.5	45
56	Actinide selectivity of 1,10-phenanthroline-2,9-dicarboxamide and its derivatives: a theoretical prediction followed by experimental validation. Dalton Transactions, 2015, 44, 1332-1340.	3.3	60
57	Significant modulation of CO adsorption on bimetallic Au19Li cluster. Chemical Physics, 2014, 428, 75-81.	1.9	22
58	Diglycolamide-functionalized task specific ionic liquids for nuclear waste remediation: extraction, luminescence, theoretical and EPR investigations. RSC Advances, 2014, 4, 46613-46623.	3.6	40
59	Structural and Chemical Properties of Subnanometer-Sized Bimetallic Au₁₉Pt Cluster. Journal of Physical Chemistry C, 2014, 118, 11935-11945.	3.1	30
60	Pu@C₂₄: A New Example Satisfying the 32-Electron Principle. Journal of Physical Chemistry C, 2014, 118, 7211-7221.	3.1	26
61	Density functional investigation on the structures and properties of Li atom doped Au₂₀ cluster. Molecular Physics, 2013, 111, 725-734.	1.7	16
62	Hydrogen bonding interaction between HO2 radical and selected organic acids, RCOOH (R=CH3, H, Cl) Tj ETQq0 0 0 rgBT /Overlock 10	2.6	5
63	Theoretical prediction of rare gas inserted hydronium ions: HRgOH2+. Journal of Chemical Physics, 2013, 138, 194308.	3.0	21
64	Structure and Stability of Zn, Cd, and Hg Atom Doped Golden Fullerene (Au₃₂). Journal of Physical Chemistry C, 2013, 117, 18777-18788.	3.1	16
65	Rational Design of Boradiazaindacene (BODIPY)â€Based Functional Molecules. Chemistry - A European Journal, 2013, 19, 17766-17772.	3.3	41
66	Theoretical Prediction of XRgCO⁺ Ions (X = F, Cl, and Rg = Ar, Kr, Xe). Journal of Physical Chemistry A, 2013, 117, 14282-14292.	2.5	31
67	Theoretical Prediction of Rare Gas Containing Hydride Cations: HRgBF⁺ (Rg = He, Ar, Kr,) Tj ETQq1 1 0.784314 rgBT /Ove	2.5	37
68	Enhancement in the Stability of 36-Atom Fullerene through Encapsulation of a Uranium Atom. Journal of Physical Chemistry C, 2013, 117, 17859-17869.	3.1	24
69	Complexation of trivalent lanthanides and actinides with several novel diglycolamide-functionalized calix[4]arenes: solvent extraction, luminescence and theoretical studies. RSC Advances, 2013, 3, 9296.	3.6	27
70	Diorgano-Gallium and -Indium Complexes Derived from Benzoazole Ligands: Synthesis, Characterization, Photoluminescence, and Computational Studies. Organometallics, 2013, 32, 104-111.	2.3	30
71	Hydrogen Bonding in Neutral and Cation Dimers of H₂Se with H₂O, H₂S, and H₂Se. Journal of Physical Chemistry A, 2012, 116, 11965-11972.	2.5	17
72	Nonlinear Optical Properties of Au₁₉M (M = Li, Na, K, Rb, Cs, Cu, Ag) Clusters. Journal of Physical Chemistry C, 2012, 116, 193-200.	3.1	24

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73	Synthesis, Characterization, Photoluminescence, and Computational Studies of Monoorgano-Gallium and -Indium Complexes Containing Dianionic Tridentate ONE (E = O or S) Schiff Bases. Organometallics, 2012, 31, 3836-3843.	2.3	25
74	Structure and binding energies of halogenated hydroxymethoxy radicalâ€“water hydrogen-bonded complexes: HOC(X)(Y)OÂ·nH2O (n=0, 1, 2 and X, Y=H/F/Cl). Computational and Theoretical Chemistry, 2012, 992, 30-36.	2.5	1
75	Theoretical Prediction of Icosahedral U@C₂₀ and Analogous Systems with High HOMOâ€“LUMO Gap. Journal of Physical Chemistry C, 2012, 116, 16716-16725.	3.1	30
76	Prediction of a New Series of Thermodynamically Stable Actinide Encapsulated Fullerene Systems Fulfilling the 32-Electron Principle. Journal of Physical Chemistry C, 2012, 116, 25630-25641.	3.1	37
77	Interesting periodic variations in physical and chemical properties of homonuclear diatomic molecules. International Journal of Quantum Chemistry, 2012, 112, 1097-1106.	2.0	10
78	Hydrogenâ€bonded complexes of nicotine with simple alcohols. International Journal of Quantum Chemistry, 2012, 112, 2787-2793.	2.0	8
79	Complexation behavior of trivalent actinides and lanthanides with 1,10-phenanthroline-2,9-dicarboxylic acid based ligands: insight from density functional theory. Physical Chemistry Chemical Physics, 2012, 14, 11060.	2.8	57
80	Polarizability, Ionization Potential, and Softness of Water and Methanol Clusters: An Interrelation. Journal of Physical Chemistry A, 2012, 116, 6831-6836.	2.5	21
81	A first-principles study of the effect of oxygen vacancy on rutile Ti1â^'xCdxO2. Solid State Communications, 2012, 152, 142-146.	1.9	1
82	Steric Strain Release-Directed Regioselective Functionalization of meso-Methyl Bodipy Dyes. Organic Letters, 2011, 13, 5870-5873.	4.6	45
83	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
84	Substituent effect on ionization potential, Oâ€“H bond dissociation energy and intra-molecular hydrogen bonding in salicylic acid derivatives. Computational and Theoretical Chemistry, 2010, 948, 47-54.	1.5	8
85	Structures and the Electronic Properties of Au₁₉X Clusters (X = Li, Na, K, Rb, Cs, Cu, and) Tj ETQq1 1 0.784314 rgBT /Over	3.1	68
86	Excited state polarizabilities of methanol clusters. Physical Chemistry Chemical Physics, 2010, 12, 2929.	2.8	14
87	Time-Dependent Density Functional Theory Calculation of Van der Waals Coefficient of Metal Clusters. , 2009, , .		0
88	The Role of Hydrogenâ€Bonding Interactions in the Ultrafast Relaxation Dynamics of the Excited States of 3â€•and 4â€Aminofluorenâ€9â€•ones. ChemPhysChem, 2009, 10, 2995-3012.	2.1	25
89	Timeâ€dependent density functional theory calculation of van der Waals coefficient of potassium clusters. International Journal of Quantum Chemistry, 2009, 109, 1376-1384.	2.0	5
90	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. Journal of Molecular Structure, 2009, 928, 46-53.	3.6	12

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91	Hydrogen bonding interaction in complexes of hydronium ion with selective chemical species. Chemical Physics Letters, 2009, 471, 36-40.	2.6	3
92	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
93	Reactions and structural investigation of chlorpromazine radical cation. Journal of Molecular Structure, 2008, 888, 401-408.	3.6	7
94	Heterocycle-Based Isomeric Chromophores with Substantially Varying NLO Properties: A New Structureâ"Property Correlation Study. Journal of Physical Chemistry A, 2008, 112, 4844-4852.	2.5	33
95	Ab Initio Studies of Properties of Small Potassium Clusters. Journal of Physical Chemistry A, 2008, 112, 12303-12311.	2.5	23
96	Significant increase in the stability of rare gas hydrides on insertion of beryllium atom. Journal of Chemical Physics, 2007, 127, 114314.	3.0	34
97	Time-dependent density functional theory calculation of van der Waals coefficient of sodium clusters. Journal of Chemical Physics, 2007, 127, 134103.	3.0	23
98	Structural Investigation of Asymmetrical Dimer Radical Cation System (H2Oâ"H2S)+:â€‰ Proton-Transferred or Hemi-Bonded?. Journal of Physical Chemistry A, 2007, 111, 2362-2367.	2.5	22
99	Ionized State of Hydroperoxy Radicalâ"Water Hydrogen-Bonded Complex:â€‰ (HO2â"H2O)+. Journal of Physical Chemistry A, 2007, 111, 13590-13594.	2.5	13
100	Hydration of uranyl cations: Effective fragment potential approach. Computational and Theoretical Chemistry, 2007, 807, 93-99.	1.5	10
101	Hydrogen Bonding in Substituted Formic Acid Dimers. Journal of Physical Chemistry A, 2006, 110, 12623-12628.	2.5	48
102	Twisting Dynamics in the Excited Singlet State of Michler's Ketone. Journal of Physical Chemistry A, 2006, 110, 3432-3446.	2.5	38
103	THEORETICAL STUDIES ON POLARIZABILITY OF ALKALI METAL CLUSTERS. , 2006, , 625-655.		0
104	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)?. Journal of Chemical Physics, 2006, 124, 124304.	3.0	77
105	Structure of thiocyanate dimer radical anion: An ab initio study. Computational and Theoretical Chemistry, 2005, 723, 235-239.	1.5	4
106	Ab initio studies on the polarizability of lithium clusters: Some unusual results. International Journal of Quantum Chemistry, 2005, 105, 166-173.	2.0	21
107	Electron Density and Energy Decomposition Analysis in Hydrogen-Bonded Complexes of Azabenzenes with Water, Acetamide, and Thioacetamide. Journal of Physical Chemistry A, 2005, 109, 7575-7582.	2.5	44
108	Insertion of noble-gas atom (Kr and Xe) into noble-metal molecules (AuF and AuOH): Are they stable?. Journal of Chemical Physics, 2005, 123, 074323.	3.0	74

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109	Ultrafast Intermolecular Hydrogen Bond Dynamics in the Excited State of Fluorenone. Journal of Physical Chemistry A, 2005, 109, 8693-8704.	2.5	100
110	Gold behaves as hydrogen: Prediction on the existence of a new class of boron-containing radicals, AuBX (X=F,Cl,Br). Journal of Chemical Physics, 2005, 123, 241101.	3.0	22
111	Static dipole polarizability and binding energy of sodium clusters Nanâ€Š(n=1â€“10): A critical assessment of all-electron based post Hartreeâ€“Fock and density functional methods. Journal of Chemical Physics, 2004, 120, 6487-6494.	3.0	58
112	Magic clusters MAu4 (M=Ti and Zr) and their dimers: How magic are they?. Journal of Chemical Physics, 2004, 120, 11363-11366.	3.0	23
113	Relationship between Ionization Potential, Polarizability, and Softness:â€‰ A Case Study of Lithium and Sodium Metal Clusters. Journal of Physical Chemistry A, 2004, 108, 6661-6666.	2.5	92
114	Reactions of Methyl Viologen Dication (MV2+) with H Atoms in Aqueous Solution:â€‰ Mechanism Derived from Pulse Radiolysis Measurements and ab Initio MO Calculations. Journal of Physical Chemistry A, 2003, 107, 5998-6006.	2.5	30
115	Hydrogen-Bonding Interactions in Selected Super-molecular Systems:â€‰ Electron Density Point of View. Journal of Physical Chemistry A, 2003, 107, 7062-7067.	2.5	20
116	Polarizability of water clusters: Anab initioinvestigation. Journal of Chemical Physics, 2003, 118, 8547-8550.	3.0	42
117	Hardness and Polarizability Profiles for Intramolecular Proton Transfer in Water Dimer Radical Cation. Journal of Physical Chemistry A, 2002, 106, 4200-4204.	2.5	44
118	Ab Initio CASSCF and DFT Investigations of (H2O)2+ and (H2S)2+:â€‰ Hemi-Bonded vs Proton-Transferred Structure. Journal of Physical Chemistry A, 2002, 106, 11815-11821.	2.5	34
119	Ab initio calculations on XFnq (X = I, Xe, Cs, and Ba;n=1, 2, 4, and 6;q=?1, 0, +1, and +2) molecules. International Journal of Quantum Chemistry, 2001, 81, 238-245.	2.0	2
120	Theoretical investigation of electronic structure and ESR hyperfine parameters for the CuH+ molecule. International Journal of Quantum Chemistry, 2000, 77, 291-300.	2.0	30
121	Molecular Hardness, Polarizability and Valency Variation of Formamide and Thioformamide on Internal Rotation:â€‰ A Density Functional Study. Journal of Physical Chemistry A, 2000, 104, 2975-2979.	2.5	27
122	Is the Hydrogen Bond in Water Dimer and Ice Covalent?. Journal of the American Chemical Society, 2000, 122, 1210-1214.	13.7	174
123	Electron spin resonance studies of 45Sc17O,â€Š89Y17O, and 139La17O in rare gas matrices: Comparison with ab initio electronic structure and nuclear hyperfine calculations. Journal of Chemical Physics, 1999, 110, 5658-5669.	3.0	40
124	Reassignment of the AlSiâ€” photoelectron spectrum by ab initio configuration interaction calculations. Molecular Physics, 1999, 96, 735-740.	1.7	3
125	Electronic Structure and Low-Lying Electronic States of Al3O and Al3O-:â€‰ Photoelectron Spectrum of Al3O-. Journal of Physical Chemistry A, 1999, 103, 2867-2872.	2.5	28
126	Theoretical Interpretation of the Photoelectron Spectra of Al3O2-and Al3O3-. Journal of Physical Chemistry A, 1999, 103, 8985-8993.	2.5	35

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127	Reassignment of the AlSi- photoelectron spectrum by ab initio configuration interaction calculations. Molecular Physics, 1999, 96, 735-740.	1.7	3
128	A peculiar excited electronic state of allene (1,2-propadiene). Chemical Physics Letters, 1998, 287, 61-69.	2.6	18
129	Proton Affinity and Acidity of Hypohalous Acids:Â A Density Functional Study. Journal of Physical Chemistry A, 1997, 101, 5022-5025.	2.5	15
130	Density functional study of the relationship between energy, hardness, and polarizability of molecules in nonequilibrium situations. International Journal of Quantum Chemistry, 1997, 63, 917-926.	2.0	6
131	A Density Functional Approach to Hardness, Polarizability, and Valency of Molecules in Chemical Reactions. The Journal of Physical Chemistry, 1996, 100, 12295-12298.	2.9	180
132	A new simple approach to the polarizability of atoms and ions using frontier orbitals from the Kohn-Sham density functional theory. Computational and Theoretical Chemistry, 1996, 366, 139-144.	1.5	9
133	Electronegativity-based approach to a new potential energy function for bond extensions. Computational and Theoretical Chemistry, 1994, 309, 143-149.	1.5	1
134	Spin-Polarized Generalization of the Concepts of Electronegativity and Hardness and the Description of Chemical Binding. Journal of the American Chemical Society, 1994, 116, 3943-3948.	13.7	89
135	Electronegativity, hardness, and chemical binding in simple molecular systems. Inorganic Chemistry, 1992, 31, 1951-1955.	4.0	33
136	A new electronegativity based approach to the calculation of partial atomic charges and other related reactivity indices in molecules. Computational and Theoretical Chemistry, 1992, 276, 83-96.	1.5	12
137	Theoretical prediction of FNgM3â€“kHk (Ngâ€‰=â€‰Ar, Kr, Xe, and Rn; Mâ€‰=â€‰Cu, Ag and Au; kâ€‰=â€‰0â€“2) molecules Molecular Physics, 0, , .	1.7	4