Pratim Kumar Chattaraj

List of Publications by Year
in descending order

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278	13,245	38742 50	29157 104
papers	citations	h-index	g-index

300	300	300	6205
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Electrophilicity Index. Chemical Reviews, 2006, 106, 2065-2091.	47.7	1,383
2	Principle of maximum hardness. Journal of the American Chemical Society, 1991, 113, 1854-1855.	13.7	1,188
3	Philicity:Â A Unified Treatment of Chemical Reactivity and Selectivity. Journal of Physical Chemistry A, 2003, 107, 4973-4975.	2.5	660
4	HSAB principle. Journal of the American Chemical Society, 1991, 113, 1855-1856.	13.7	569
5	Update 1 of: Electrophilicity Index. Chemical Reviews, 2007, 107, PR46-PR74.	47.7	509
6	Update 2 of: Electrophilicity Index. Chemical Reviews, 2011, 111, PR43-PR75.	47.7	286
7	Variation of the Electrophilicity Index along the Reaction Path. Journal of Physical Chemistry A, 2003, 107, 7068-7072.	2.5	263
8	Conceptual density functional theory: status, prospects, issues. Theoretical Chemistry Accounts, 2020, 139, 1.	1.4	249
9	Stability, Reactivity, and Aromaticity of Compounds of a Multivalent Superatom. Journal of Physical Chemistry A, 2007, 111, 11116-11121.	2.5	218
10	Electrophilicity index within a conceptual DFT framework. Annual Reports on the Progress of Chemistry Section C, 2009, 105, 13.	4.4	181
11	The maximum hardness principle in the Gyftopoulos-Hatsopoulos three-level model for an atomic or molecular species and its positive and negative ions. Chemical Physics Letters, 1995, 237, 171-176.	2.6	177
12	Net Electrophilicity. Journal of Physical Chemistry A, 2009, 113, 10068-10074.	2.5	173
13	HSAB Principle Applied to the Time Evolution of Chemical Reactionsâ€. Journal of the American Chemical Society, 2003, 125, 2705-2710.	13.7	163
14	The Woodwardâ€“Hoffmann Rules Reinterpreted by Conceptual Density Functional Theory. Accounts of Chemical Research, 2012, 45, 683-695.	15.6	156
15	An ab initio study resulting in a greater understanding of the HSAB principle. Journal of the American Chemical Society, 1994, 116, 1067-1071.	13.7	153
16	On the Validity of the Maximum Hardness Principle and the Minimum Electrophilicity Principle during Chemical Reactions. Journal of Physical Chemistry A, 2013, 117, 1843-1852.	2.5	152
17	Variational method for determining the Fukui function and chemical hardness of an electronic system. Journal of Chemical Physics, 1995, 103, 7645-7646.	3.0	138
18	A comparative study to predict regioselectivity, electrophilicity and nucleophilicity with Fukui function and Hirshfeld charge. Theoretical Chemistry Accounts, 2019, 138, 1.	1.4	138

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19	Is the Fukui Function a Right Descriptor of Hardâ^'Hard Interactions?. Journal of Physical Chemistry A, 2004, 108, 2487-2491.	2.5	131
20	Aspects of the Softness and Hardness Concepts of Densityâ€Functional Theory. Israel Journal of Chemistry, 1991, 31, 395-402.	2.3	128
21	Validity of the Minimum Polarizability Principle in Molecular Vibrations and Internal Rotations:Â An ab Initio SCF Study. Journal of Physical Chemistry A, 1999, 103, 9307-9312.	2.5	127
22	Hydrogen Storage in Clathrate Hydrates. Journal of Physical Chemistry A, 2011, 115, 187-193.	2.5	110
23	B₁₈^{2â^'}: a quasi-planar bowl member of the Wankel motor family. Chemical Communications, 2014, 50, 8140-8143.	4.1	107
24	The maximum hardness principle implies the hard/soft acid/base rule. Journal of Chemical Physics, 2005, 123, 086101.	3.0	100
25	Conceptual density functional theory based electronic structure principles. Chemical Science, 2021, 12, 6264-6279.	7.4	96
26	Local hardness: a critical account. Theoretical Chemistry Accounts, 2007, 118, 923-930.	1.4	95
27	Molecular Electronic Excitations and the Minimum Polarizability Principle. Journal of Physical Chemistry A, 2000, 104, 3185-3187.	2.5	94
28	Woodwardâ^'Hoffmann Rule in the Light of the Principles of Maximum Hardness and Minimum Polarizability:Â DFT and Ab Initio SCF Studies. Journal of the American Chemical Society, 2000, 122, 348-351.	13.7	90
29	Fukui function from a gradient expansion formula, and estimate of hardness and covalent radius for an atom. Journal of Chemical Physics, 1995, 103, 10621-10626.	3.0	89
30	Further links between the maximum hardness principle and the hard/soft acid/base principle: insights from hard/soft exchange reactions. Physical Chemistry Chemical Physics, 2007, 9, 3853.	2.8	89
31	Dynamical behavior of Borospherene: A Nanobubble. Scientific Reports, 2015, 5, 11287.	3.3	81
32	Ring Expansion of Donorâ€“Acceptor Cyclopropane via Substituent Controlled Selective N-Transfer of Oxaziridine: Synthetic and Mechanistic Insights. Organic Letters, 2016, 18, 4940-4943.	4.6	73
33	The hydrogen trapping potential of some Li-doped star-like clusters and super-alkali systems. Physical Chemistry Chemical Physics, 2012, 14, 10345.	2.8	71
34	Understanding local electrophilicity/nucleophilicity activation through a single reactivity difference index. Organic and Biomolecular Chemistry, 2012, 10, 2855.	2.8	68
35	In Quest of Strong Beâ€“Ng Bonds among the Neutral Ngâ€“Be Complexes. Journal of Physical Chemistry A, 2014, 118, 487-494.	2.5	68
36	Ab Initio SCF and DFT Studies on Solvent Effects on Intramolecular Rearrangement Reactions. Journal of Physical Chemistry A, 2001, 105, 4272-4283.	2.5	67

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37	Structure and bonding of IrB₁₂^{â^'}: converting a rigid boron B₁₂ platelet to a Wankel motor. RSC Advances, 2016, 6, 27177-27182.	3.6	67
38	Appraisal of Chemical Bond Making, Bond Breaking, and Electron Transfer in Solution in the Light of the Principle of Maximum Hardness. Journal of Organic Chemistry, 1995, 60, 4707-4714.	3.2	65
39	Scaling properties of information-theoretic quantities in density functional reactivity theory. Physical Chemistry Chemical Physics, 2015, 17, 4977-4988.	2.8	65
40	Unprecedented Bonding Situation in Viable E₂(NHB^{Me})₂ (E=Be,) Tj ETQq0 0 0 rgBT /Overlock 10 Forms a Single Eâ^'E Covalent Bond. Angewandte Chemie - International Edition, 2019, 58, 8372-8377.	13.8	62
41	Confinement induced binding of noble gas atoms. Journal of Chemical Physics, 2014, 140, 164306.	3.0	61
42	Pyrrole-Based New Diphosphines: Pd and Ni Complexes Bearing the PNP Pincer Ligand. Inorganic Chemistry, 2012, 51, 12527-12539.	4.0	60
43	Atoms-in-molecules partitioning of a molecular density. International Journal of Quantum Chemistry, 2000, 77, 403-407.	2.0	58
44	Chemical softness in model electronic systems: dependence on temperature and chemical potential. Chemical Physics, 1996, 204, 429-437.	1.9	57
45	Reactivity, Selectivity, and Aromaticity of Be₃²⁻ and Its Complexes. Journal of Physical Chemistry A, 2008, 112, 1612-1621.	2.5	57
46	Electrophilicity Equalization Principle. Journal of Physical Chemistry Letters, 2010, 1, 1064-1067.	4.6	57
47	Synthesis, structure and electrochemical behaviour of Ru(ii)- and Pt(ii)-carbene complexes of the NCN-pincer 1,3-bis(2-pyridylmethyl)-1H-benzimidazolium chloride. New Journal of Chemistry, 2010, 34, 1974.	2.8	57
48	A Cu(ii)-MOF capable of fixing CO2 from air and showing high capacity H2 and CO2 adsorption. Chemical Communications, 2017, 53, 13371-13374.	4.1	57
49	Comparison between the frozen core and finite differences approximations for the generalized spin-dependent global and local reactivity descriptors in small molecules. Theoretical Chemistry Accounts, 2006, 115, 257-265.	1.4	53
50	Aromaticity in Polyacene Analogues of Inorganic Ring Compounds. Journal of Physical Chemistry A, 2007, 111, 4684-4696.	2.5	52
51	Cucurbit[6]uril: A Possible Host for Noble Gas Atoms. Journal of Physical Chemistry B, 2015, 119, 10962-10974.	2.6	50
52	C₅Li₇⁺ and O₂Li₅⁺ as Nobleâ€Gasâ€Trapping Agents. Chemistry - A European Journal, 2013, 19, 2322-2329.	3.3	49
53	Metastable behavior of noble gas inserted tin and lead fluorides. Physical Chemistry Chemical Physics, 2015, 17, 972-982.	2.8	49
54	Selectivity in Gas Adsorption by Molecular Cucurbit[6]uril. Journal of Physical Chemistry C, 2016, 120, 13911-13921.	3.1	49

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55	Ïƒ-Aromatic cyclic M₃⁺ (M = Cu, Ag, Au) clusters and their complexation with dimethyl imidazol-2-ylidene, pyridine, isoxazole, furan, noble gases and carbon monoxide. Physical Chemistry Chemical Physics, 2016, 18, 11661-11676.	2.8	49
56	Bonding, Reactivity, and Dynamics in Confined Systems. Journal of Physical Chemistry A, 2019, 123, 4513-4531.	2.5	48
57	Chemical bonding and reactivity: a local thermodynamic viewpoint. Chemical Physics Letters, 1999, 314, 114-121.	2.6	47
58	Comparative Study on the Noble-Gas Binding Ability of BeX Clusters (X = SO₄,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 622 T	2.5	47
59	Density functional theory of chemical hardness. , 1993, , 11-25.		45
60	Aromaticity and antiaromaticity of substituted fulvene derivatives: perspectives from the information-theoretic approach in density functional reactivity theory. Physical Chemistry Chemical Physics, 2017, 19, 18635-18645.	2.8	43
61	Is It Possible To Determine Oxidation States for Atoms in Molecules Using Density-Based Quantities? An Information-Theoretic Approach and Conceptual Density Functional Theory Study. Journal of Physical Chemistry A, 2019, 123, 6751-6760.	2.5	43
62	Towards understanding the molecular internal rotations and vibrations and chemical reactions through the profiles of reactivity and selectivity indices: an ab initio SCF and DFT study. Molecular Physics, 2003, 101, 2841-2853.	1.7	42
63	Nobleâ€Noble Strong Union: Gold at Its Best to Make a Bond with a Noble Gas Atom. ChemistryOpen, 2019, 8, 173-187.	1.9	42
64	Structure and Stability of (NG)_nCN₃Be₃⁺ Clusters and Comparison with (NG)BeY^{0/+}. ChemPhysChem, 2013, 14, 2511-2517.	2.1	41
65	A coupledâ€cluster study on the noble gas binding ability of metal cyanides versus metal halides (metalâ€‰=â€‰Cu, Ag, Au). Journal of Computational Chemistry, 2015, 36, 2168-2176.	3.3	41
66	Planar pentacoordinate carbon in CGa₅⁺ derivatives. Physical Chemistry Chemical Physics, 2018, 20, 12350-12355.	2.8	41
67	Noble gas encapsulated B₄₀ cage. Physical Chemistry Chemical Physics, 2018, 20, 1953-1963.	2.8	41
68	A Density Functional Study of the Claisen Rearrangement of Allyl Aryl Ether, Allyl Arylamine, Allyl Aryl Thio Ether, and a Series of Meta-Substituted Molecules through Reactivity and Selectivity Profiles. Journal of Physical Chemistry A, 2002, 106, 11227-11233.	2.5	40
69	A tug-of-war between electronic excitation and confinement in a dynamical context. Physical Chemistry Chemical Physics, 2012, 14, 1716-1727.	2.8	40
70	Noble gas supported B₃⁺ cluster: formation of strong covalent noble gasâ€“boron bonds. RSC Advances, 2016, 6, 78611-78620.	3.6	40
71	Movement of Ng 2 molecules confined in a C 60 cage: An ab initio molecular dynamics study. Chemical Physics Letters, 2014, 610-611, 351-356.	2.6	39
72	Electron Affinity, Electronegativity, and Electrophilicity of Atoms and Ions. Journal of Chemical & Engineering Data, 2010, 55, 1882-1886.	1.9	38

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73	Analyzing the efficiency of M n â€“(C2H4) (MÂ=ÂSc, Ti, Fe, Ni; nÂ=Â1, 2) complexes as effective hydrogen storage materials. Structural Chemistry, 2011, 22, 823-837.	2.0	38
74	Exploring the Nature of Silicon-Noble Gas Bonds in H3SiNgNSi and HSiNgNSi Compounds (Ng = Xe, Rn). International Journal of Molecular Sciences, 2015, 16, 6402-6418.	4.1	37
75	Synthesis, structure and theoretical studies of Hg(II)â€“NH carbene complex of annulated ligand pyridinyl[1,2-a]{2-pyridylimidazol}-3-ylidene hexaflurophosphate. Inorganica Chimica Acta, 2011, 375, 271-279.	2.4	36
76	Stability of Nobleâ€Gasâ€Bound SiH₃⁺ Clusters. ChemPhysChem, 2014, 15, 3554-3564.	2.1	36
77	Ab Initio Study on the Stability of Ng_nBe₂N₂, Ng_nBe₃N₂ and NgBeSiN₂ Clusters. ChemPhysChem, 2014, 15, 2618-2625.	2.1	35
78	Two Closely Related Zn(II)-MOFs for Their Large Difference in CO₂ Uptake Capacities and Selective CO₂ Sorption. Inorganic Chemistry, 2020, 59, 7056-7066.	4.0	35
79	A computational study on the hydrogen adsorption capacity of various lithiumâ”Doped boron hydrides. Journal of Computational Chemistry, 2012, 33, 425-434.	3.3	34
80	How strong are the metalloceneâ€“metallocene interactions? Cases of ferrocene, ruthenocene, and osmocene. Physical Chemistry Chemical Physics, 2016, 18, 550-556.	2.8	34
81	Confinement induced thermodynamic and kinetic facilitation of some Dielsâ€“Alder reactions inside a CB[7] cavitand. Journal of Computational Chemistry, 2018, 39, 151-160.	3.3	34
82	How Far Can One Push the Noble Gases Towards Bonding?: A Personal Account. Molecules, 2019, 24, 2933.	3.8	34
83	Reactivity Dynamics. Journal of Physical Chemistry A, 2021, 125, 2051-2060.	2.5	34
84	Scrutiny of the HSAB Principle in Some Representative Acidâ”Base Reactions. Journal of Physical Chemistry A, 2001, 105, 8815-8820.	2.5	33
85	Confinement induced binding in noble gas atoms within a BN-doped carbon nanotube. Chemical Physics Letters, 2015, 621, 29-34.	2.6	33
86	Finite temperature grand canonical ensemble study of the minimum electrophilicity principle. Journal of Chemical Physics, 2017, 147, 124103.	3.0	33
87	Synthesis and structure of 1-D Na6cluster chain with short Naâ€“Na distance: Organic like aromaticity in inorganic metal cluster. Chemical Communications, 2007, , 135-137.	4.1	32
88	Cyanideâ€“isocyanide isomerization: stability and bonding in noble gas inserted metal cyanides (metal =) Tj ETQq0 0 0 rgBT /Overlock 1	2.8	32
89	Local Descriptors around a Transition State:â€‰ A Link between Chemical Bonding and Reactivity. Journal of Physical Chemistry A, 2005, 109, 3771-3772.	2.5	31
90	Minimum magnetizability principle. Journal of Chemical Physics, 2006, 125, 056101.	3.0	31

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91	Noble gas encapsulation: clathrate hydrates and their HF doped analogues. Physical Chemistry Chemical Physics, 2014, 16, 17943-17954.	2.8	31
92	A Spinning Umbrella: Carbon Monoxide and Dinitrogen Bound MB₁₂^{â€“} Clusters (M = Co, Rh, Ir). Journal of Physical Chemistry A, 2017, 121, 2971-2979.	2.5	31
93	Low Operating Voltage Organic Field-Effect Transistors with Gelatin as a Moisture-Induced Ionic Dielectric Layer: The Issues of High Carrier Mobility. ACS Applied Materials & Interfaces, 2020, 12, 19727-19736.	8.0	31
94	Trapping of noble gases (Heâ€“Kr) by the aromatic H3+ and Li3+ species: a conceptual DFT approach. New Journal of Chemistry, 2010, 34, 1936.	2.8	30
95	Potential use of some metal clusters as hydrogen storage materialsâ€”a conceptual DFT approach. Journal of Molecular Modeling, 2011, 17, 777-784.	1.8	30
96	A (Tâ€“P) Phase Diagram of Hydrogen Storage on (N₄C₃H)₆Li₆. Journal of Physical Chemistry A, 2012, 116, 3259-3266.	2.5	30
97	Cucurbiturils as promising hydrogen storage materials: a case study of cucurbit[7]uril. New Journal of Chemistry, 2013, 37, 2492.	2.8	30
98	Biological Activity and Toxicity: A Conceptual DFT Approach. Structure and Bonding, 2013, , 143-179.	1.0	29
99	Encapsulation of small gas molecules and rare gas atoms inside the octa acid cavitand. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	29
100	Theoretical study of the trans-N2H2â†'cis-N2H2 and F2S2â†'FSSF reactions in gas and solution phases.. Computational and Theoretical Chemistry, 2002, 580, 171-182.	1.5	28
101	A Possible Union of Chemical Bonding, Reactivity, and Kinetics. Journal of Physical Chemistry A, 2006, 110, 11401-11403.	2.5	28
102	Bonding and aromaticity in an all-metal sandwich-like compound, <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" display="inline" overflow="scroll"><mml:mrow><mml:msubsup><mml:mrow><mml:mtext>Be</mml:mtext></mml:mrow><mml:mrow><mml:mn>8</mml:mn></mml:mrow> Chemical Physics Letters, 2008, 460, 382-385.	2.6	28
103	Structure and stability of noble gas bound compounds (Eâ€‰=â€‰C, Ge, Sn, Pb; Xâ€‰=â€‰H, F, Cl, Br). Journal of Computational Chemistry, 2016, 37, 226-236.	3.3	28
104	Modified Particle Swarm Optimization Algorithms for the Generation of Stable Structures of Carbon Clusters, Cn (n = 3â€“6, 10). Frontiers in Chemistry, 2019, 7, 485.	3.6	28
105	Electrophilicity index revisited. Journal of Computational Chemistry, 2023, 44, 278-297.	3.3	28
106	Bonding, aromaticity, and structure of trigonal dianion metal clusters. Journal of Computational Chemistry, 2010, 31, 1815-1821.	3.3	27
107	On the stability of noble gas bound 1-tris(pyrazolyl)borate beryllium and magnesium complexes. New Journal of Chemistry, 2015, 39, 6778-6786.	2.8	27
108	A computational study on structure, stability and bonding in Noble Gas bound metal Nitrates, Sulfates and Carbonates (Metal = Cu, Ag, Au). Journal of Chemical Sciences, 2016, 128, 1537-1548.	1.5	27

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109	MNgCCH (M = Cu, Ag, Au; Ng = Xe, Rn): The First Set of Compounds with Mâ€“Ngâ€“C Bonding Motif. Journal of Physical Chemistry A, 2017, 121, 6491-6499.	2.5	27
110	A theoretical investigation on boronâ€“ligand cooperation to activate molecular hydrogen by a frustrated Lewis pair and subsequent reduction of carbon dioxide. Physical Chemistry Chemical Physics, 2019, 21, 21267-21277.	2.8	27
111	Aromaticity in cyclic alkali clusters. Physical Chemistry Chemical Physics, 2008, 10, 2461.	2.8	26
112	Attractive Xeâ€“Li interaction in Li-decorated clusters. Computational and Theoretical Chemistry, 2013, 1021, 62-69.	2.5	26
113	Reactivity dynamics of a confined molecule in presence of an external magnetic field. International Journal of Quantum Chemistry, 2015, 115, 144-157.	2.0	26
114	A noble interaction: An assessment of noble gas binding ability of metal oxides (metalâ€‰=â€‰Cu, Ag, Au). International Journal of Quantum Chemistry, 2016, 116, 1016-1024.	2.0	26
115	Optical response and gas sequestration properties of metal cluster supported graphene nanoflakes. Physical Chemistry Chemical Physics, 2016, 18, 18811-18827.	2.8	26
116	Noble Gas Inserted Metal Acetylides (Metal = Cu, Ag, Au). Journal of Physical Chemistry A, 2018, 122, 7391-7401.	2.5	25
117	Metalâ€“Organic Frameworks of Cu(II) Constructed from Functionalized Ligands for High Capacity H₂ and CO₂ Gas Adsorption and Catalytic Studies. Inorganic Chemistry, 2020, 59, 1810-1822.	4.0	25
118	Role of aromaticity and charge of a system in its hydrogen trapping potential and vice versa. Physical Chemistry Chemical Physics, 2011, 13, 20602.	2.8	24
119	Pd(II)â€“N-heterocyclic carbene complexes of 2,6-bis{N-methyl-(imidazolium/benzimidazolium)}pyrazinechloride: Synthesis, structure, catalysis and theoretical studies. Inorganica Chimica Acta, 2012, 383, 83-90.	2.4	24
120	Does Confinement Always Lead to Thermodynamically and/or Kinetically Favorable Reactions? A Case Study using Dielsâ€“Alder Reactions within ExBox⁺⁴ and CB[7]. ChemPhysChem, 2017, 18, 2162-2170.	2.1	24
121	Local hardness equalization and the principle of maximum hardness. Journal of Chemical Physics, 2013, 138, 214103.	3.0	23
122	In Quest of a Superhalogen Supported Covalent Bond Involving a Noble Gas Atom. Journal of Physical Chemistry A, 2015, 119, 3064-3074.	2.5	23
123	A computational study on hydrogenation of CO2, catalyzed by a bridged B/N frustrated Lewis pair. Structural Chemistry, 2019, 30, 1067-1077.	2.0	23
124	Aromaticity and hydrogen storage capability of planar and rings. Chemical Physics Letters, 2011, 506, 315-320.	2.6	22
125	Toward analyzing some neutral and cationic boronâ€“lithium clusters (B_xLi_y x = 2â€“6; y = 1, 2) as effective hydrogen storage materials: A conceptual density functional study. International Journal of Quantum Chemistry, 2012, 112, 695-702.	2.0	22
126	Unprecedented Bonding Situation in Viable E₂(NHB^{Me})₂ (E=Be,) Tj ETQq0 0 0 rgBT /Overlock 10 Forms a Single Eâ˜E Covalent Bond. Angewandte Chemie, 2019, 131, 8460-8465.	2.0	22

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127	A new healable polymer material based on ultrafast Dielsâ€“Alder â€˜clickâ€™ chemistry using triazolinedione and fluorescent anthracyl derivatives: a mechanistic approach. Polymer Chemistry, 2019, 10, 5070-5079.	3.9	21
128	Aromaticity in all-metal annular systems: the counter-ion effect. Physical Chemistry Chemical Physics, 2011, 13, 14865.	2.8	20
129	Reactivity dynamics of confined atoms in the presence of an external magnetic field. European Physical Journal D, 2014, 68, 1.	1.3	20
130	DFT study on the ground state and excited state intramolecular proton transfer of propargyl arm containing Schiff bases in solution and gas phases. Computational and Theoretical Chemistry, 2014, 1028, 19-26.	2.5	20
131	Noble gas bound beryllium chromate and beryllium hydrogen phosphate: a comparison with noble gas bound beryllium oxide. RSC Advances, 2016, 6, 92786-92794.	3.6	20
132	Stable NCNgNSi (Ng=Kr, Xe, Rn) Compounds with Covalently Bound Câ€Ngâ€N Unit: Possible Isomerization of NCNSi through the Release of the Noble Gas Atom. Chemistry - A European Journal, 2018, 24, 2879-2887.	3.3	20
133	Encapsulation of Mg₂ inside a C₆₀ cage forms an electride. Journal of Computational Chemistry, 2020, 41, 1645-1653.	3.3	20
134	Acidity of meta- and para-substituted aromatic acids: a conceptual DFT study. New Journal of Chemistry, 2008, 32, 1945.	2.8	19
135	A one-pot Garrattâ€“Braverman cyclization and Scholl oxidation route to aceneâ€“helicene hybrids. RSC Advances, 2013, 3, 19844.	3.6	19
136	Hostâ€“Guest Interactions in ExBox⁴⁺. ChemPhysChem, 2014, 15, 4108-4116.	2.1	19
137	The strongest CO binding and the highest Câ€“O stretching frequency. Physical Chemistry Chemical Physics, 2017, 19, 2286-2293.	2.8	19
138	Boron Nanowheels with Axles Containing Noble Gas Atoms: Viable Noble Gas Bound MÂ©B₁₀^{â^'} Clusters (M=Nb, Ta). Chemistry - A European Journal, 2018, 24, 3590-3598.	3.3	19
139	Filling the void: controlled donorâ€“acceptor interaction facilitates the formation of an Mâ€“M single bond in the zero oxidation state of M (M = Zn, Cd, Hg). Dalton Transactions, 2020, 49, 1056-1064.	3.3	19
140	Activation of Small Molecules and Hydrogenation of CO2 Catalyzed by Frustrated Lewis Pairs. Catalysts, 2022, 12, 201.	3.5	19
141	Noble Gas Binding Ability of Metalâ€Bipyridine Monocationic Complexes (Metal=Cu, Ag, Au): A Computational Study. ChemistrySelect, 2016, 1, 5842-5849.	1.5	18
142	Hydrophobicity versus electrophilicity: A new protocol toward quantitative structureâ€“toxicity relationship. Chemical Biology and Drug Design, 2019, 93, 1083-1095.	3.2	18
143	Cycloaddition Reactions between H₂C = CHR (R = H, CN, CH₃) and a Cyclic P/B Frustrated Lewis Pair: A DFT Study. Journal of Physical Chemistry A, 2020, 124, 4455-4462.	2.5	18
144	Exchange?correlation potential and excited-state density functional theory. International Journal of Quantum Chemistry, 1996, 60, 535-543.	2.0	17

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145	Stability and aromaticity of nH₂@B₁₂N₁₂(n=1â€“12) clusters. Nano Reviews, 2011, 2, 5767.	3.7	17
146	Analyzing torquoselectivity in electrocyclic ring opening reactions of trans-3,4-dimethylcyclobutene and 3-formylcyclobutene through electronic structure principles. Physical Chemistry Chemical Physics, 2015, 17, 23104-23111.	2.8	17
147	Stabilization of Boronâ€“Boron Triple Bonds by Mesoionic Carbenes. ACS Omega, 2018, 3, 13720-13730.	3.5	17
148	Quantitative structureâ€toxicity relationship: An â€œin silico studyâ€•using electrophilicity and hydrophobicity as descriptors. International Journal of Quantum Chemistry, 2020, 120, e26097.	2.0	17
149	Electride Characteristics of Some Binuclear Sandwich Complexes of Alkaline Earth Metals, M₂(Î·⁵-L)₂(M = Be, Mg; L =) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 582 Td (C₅	2.5	17
150	Flexibility Induced Encapsulation of Ultrafine Palladium Nanoparticles into Organic Cages for Tsujiâ€“Trost Allylation. ACS Applied Materials & Interfaces, 2020, 12, 8539-8546.	8.0	17
151	Local Temperature as a Chemical Reactivity Descriptor. Journal of Physical Chemistry Letters, 2021, 12, 5623-5630.	4.6	17
152	A philicity based analysis of adsorption of small molecules in zeolites. Journal of Chemical Sciences, 2005, 117, 541-548.	1.5	16
153	Comment on â€œRuling Out Any Electrophilicity Equalization Principleâ€• Journal of Physical Chemistry A, 2012, 116, 790-791.	2.5	16
154	Electrophilicity kernel and its hierarchy through softness in conceptual density functional theory. International Journal of Quantum Chemistry, 2013, 113, 2163-2171.	2.0	16
155	Chemical reactivity through structure-stability landscape. International Journal of Quantum Chemistry, 2014, 114, 1421-1429.	2.0	16
156	Binding of Small Gas Molecules by Metalâ€“Bipyridyl Monocationic Complexes (Metal = Cu, Ag, Au) and Possible Bond Activations Therein. Journal of Physical Chemistry A, 2017, 121, 3803-3817.	2.5	16
157	In Silico Studies on Selected Neutral Molecules, CGa2Ge2, CAlGaGe2, and CSiGa2Ge Containing Planar Tetracoordinate Carbon. Atoms, 2021, 9, 65.	1.6	16
158	Arsenic toxicity: an atom counting and electrophilicity-based protocol. Molecular Diversity, 2009, 13, 551-556.	3.9	15
159	HNgBeF₃ (Ngâ€‰=â€‰Arâ€Rn): Superhalogenâ€supported noble gas insertion compounds. International Journal of Quantum Chemistry, 2018, 118, e25499.	2.0	15
160	A Complex Containing Four Magnesium Atoms and Two Mgâ€“Mg Bonds Behaving as an Electride. European Journal of Inorganic Chemistry, 2019, 2019, 4105-4111.	2.0	15
161	Chemical reactivity from a conceptual density functional theory perspective. Journal of the Indian Chemical Society, 2021, 98, 100008.	2.8	15
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