# Pratim Kumar Chattaraj

## List of Publications by Citations



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| 277 papers | 10,328 citations | 45 h-index | 93 g-index |
| 300 ext. papers | 11,800 ext. citations | 4.1 avg, IF | 6.73 L-index |

| # | Paper | IF | Citations |
|---|---|---|---|
| 277 | Electrophilicity index. *Chemical Reviews*, **2006**, 106, 2065-91 | 68.1 | 1155 |
| 276 | Principle of maximum hardness. *Journal of the American Chemical Society*, **1991**, 113, 1854-1855 | 16.4 | 1025 |
| 275 | Philicity: A Unified Treatment of Chemical Reactivity and Selectivity. *Journal of Physical Chemistry A* , **2003**, 107, 4973-4975 | 2.8 | 555 |
| 274 | HSAB principle. *Journal of the American Chemical Society*, **1991**, 113, 1855-1856 | 16.4 | 502 |
| 273 | Update 1 of: Electrophilicity Index. *Chemical Reviews*, **2007**, 107, PR46-PR74 | 68.1 | 256 |
| 272 | Update 2 of: electrophilicity index. *Chemical Reviews*, **2011**, 111, PR43-75 | 68.1 | 233 |
| 271 | Variation of the Electrophilicity Index along the Reaction Path. *Journal of Physical Chemistry A*, **2003** , 107, 7068-72 | 2.8 | 212 |
| 270 | Stability, reactivity, and aromaticity of compounds of a multivalent superatom. *Journal of Physical Chemistry A*, **2007**, 111, 11116-21 | 2.8 | 185 |
| 269 | 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 | 2.5 | 163 |
| 268 | Electrophilicity index within a conceptual DFT framework. *Annual Reports on the Progress of Chemistry Section C*, **2009**, 105, 13 | | 143 |
| 267 | HSAB principle applied to the time evolution of chemical reactions. *Journal of the American Chemical Society*, **2003**, 125, 2705-10 | 16.4 | 142 |
| 266 | An ab initio study resulting in a greater understanding of the HSAB principle. *Journal of the American Chemical Society*, **1994**, 116, 1067-1071 | 16.4 | 137 |
| 265 | Net electrophilicity. *Journal of Physical Chemistry A*, **2009**, 113, 10068-74 | 2.8 | 123 |
| 264 | Variational method for determining the Fukui function and chemical hardness of an electronic system. *Journal of Chemical Physics*, **1995**, 103, 7645-7646 | 3.9 | 122 |
| 263 | On the validity of the maximum hardness principle and the minimum electrophilicity principle during chemical reactions. *Journal of Physical Chemistry A*, **2013**, 117, 1843-52 | 2.8 | 121 |
| 262 | The Woodward-Hoffmann rules reinterpreted by conceptual density functional theory. *Accounts of Chemical Research*, **2012**, 45, 683-95 | 24.3 | 119 |
| 261 | Aspects of the Softness and Hardness Concepts of Density-Functional Theory. *Israel Journal of Chemistry*, **1991**, 31, 395-402 | 3.4 | 117 |

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| 260 | Is the Fukui Function a Right Descriptor of HardHard Interactions?. *Journal of Physical Chemistry A*, **2004**, 108, 2487-2491 | 2.8 | 115 |
| 259 | Conceptual density functional theory: status, prospects, issues. *Theoretical Chemistry Accounts*, **2020**, 139, 1 | 1.9 | 113 |
| 258 | Validity of the Minimum Polarizability Principle in Molecular Vibrations and Internal Rotations: An ab Initio SCF Study. *Journal of Physical Chemistry A*, **1999**, 103, 9307-9312 | 2.8 | 112 |
| 257 | Hydrogen storage in clathrate hydrates. *Journal of Physical Chemistry A*, **2011**, 115, 187-93 | 2.8 | 99 |
| 256 | B18(2-): a quasi-planar bowl member of the Wankel motor family. *Chemical Communications*, **2014**, 50, 8140-3 | 5.8 | 98 |
| 255 | The maximum hardness principle implies the hard/soft acid/base rule. *Journal of Chemical Physics*, **2005**, 123, 086101 | 3.9 | 88 |
| 254 | Molecular Electronic Excitations and the Minimum Polarizability Principle. *Journal of Physical Chemistry A*, **2000**, 104, 3185-3187 | 2.8 | 86 |
| 253 | Local hardness: a critical account. *Theoretical Chemistry Accounts*, **2007**, 118, 923-930 | 1.9 | 80 |
| 252 | WoodwardHoffmann Rule in the Light of the Principles of Maximum Hardness and Minimum Polarizability: DFT and Ab Initio SCF Studies. *Journal of the American Chemical Society*, **2000**, 122, 348-351 | 16.4 | 80 |
| 251 | 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 | 3.9 | 78 |
| 250 | 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, 3853-6 | 3.6 | 77 |
| 249 | Dynamical behavior of Borospherene: A Nanobubble. *Scientific Reports*, **2015**, 5, 11287 | 4.9 | 70 |
| 248 | Ring Expansion of Donor-Acceptor Cyclopropane via Substituent Controlled Selective N-Transfer of Oxaziridine: Synthetic and Mechanistic Insights. *Organic Letters*, **2016**, 18, 4940-4943 | 6.2 | 67 |
| 247 | 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 | 4.2 | 60 |
| 246 | Scaling properties of information-theoretic quantities in density functional reactivity theory. *Physical Chemistry Chemical Physics*, **2015**, 17, 4977-88 | 3.6 | 59 |
| 245 | The hydrogen trapping potential of some Li-doped star-like clusters and super-alkali systems. *Physical Chemistry Chemical Physics*, **2012**, 14, 10345-50 | 3.6 | 59 |
| 244 | Ab Initio SCF and DFT Studies on Solvent Effects on Intramolecular Rearrangement Reactions. *Journal of Physical Chemistry A*, **2001**, 105, 4272-4283 | 2.8 | 59 |
| 243 | In quest of strong Be-Ng bonds among the neutral Ng-Be complexes. *Journal of Physical Chemistry A*, **2014**, 118, 487-94 | 2.8 | 57 |

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| 242 | Structure and bonding of IrB12− converting a rigid boron B12 platelet to a Wankel motor. *RSC Advances*, **2016**, 6, 27177-27182 | 3.7 | 56 |
| 241 | Reactivity, selectivity, and aromaticity of Be3(2-) and its complexes. *Journal of Physical Chemistry A*, **2008**, 112, 1612-21 | 2.8 | 53 |
| 240 | Atoms-in-molecules partitioning of a molecular density. *International Journal of Quantum Chemistry* , **2000**, 77, 403-407 | 2.1 | 53 |
| 239 | Pyrrole-based new diphosphines: Pd and Ni complexes bearing the PNP pincer ligand. *Inorganic Chemistry*, **2012**, 51, 12527-39 | 5.1 | 51 |
| 238 | A comparative study to predict regioselectivity, electrophilicity and nucleophilicity with Fukui function and Hirshfeld charge. *Theoretical Chemistry Accounts*, **2019**, 138, 1 | 1.9 | 50 |
| 237 | Confinement induced binding of noble gas atoms. *Journal of Chemical Physics*, **2014**, 140, 164306 | 3.9 | 48 |
| 236 | 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 | 1.9 | 48 |
| 235 | A Cu(ii)-MOF capable of fixing CO from air and showing high capacity H and CO adsorption. *Chemical Communications*, **2017**, 53, 13371-13374 | 5.8 | 47 |
| 234 | 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 | 3.6 | 47 |
| 233 | Understanding local electrophilicity/nucleophilicity activation through a single reactivity difference index. *Organic and Biomolecular Chemistry*, **2012**, 10, 2855-61 | 3.9 | 46 |
| 232 | Metastable behavior of noble gas inserted tin and lead fluorides. *Physical Chemistry Chemical Physics*, **2015**, 17, 972-82 | 3.6 | 45 |
| 231 | Electrophilicity Equalization Principle. *Journal of Physical Chemistry Letters*, **2010**, 1, 1064-1067 | 6.4 | 44 |
| 230 | Aromaticity in polyacene analogues of inorganic ring compounds. *Journal of Physical Chemistry A*, **2007**, 111, 4684-96 | 2.8 | 44 |
| 229 | C5Li7(+) and O2Li5(+) as noble-gas-trapping agents. *Chemistry - A European Journal*, **2013**, 19, 2322-9 | 4.8 | 43 |
| 228 | Chemical softness in model electronic systems: dependence on temperature and chemical potential. *Chemical Physics*, **1996**, 204, 429-437 | 2.3 | 42 |
| 227 | 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, 11661-76 | 3.6 | 41 |
| 226 | Cucurbit[6]uril: A Possible Host for Noble Gas Atoms. *Journal of Physical Chemistry B*, **2015**, 119, 10962-74 | 3.4 | 41 |
| 225 | Chemical bonding and reactivity: a local thermodynamic viewpoint. *Chemical Physics Letters*, **1999**, 314, 114-121 | 2.5 | 41 |

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| 224 | Unprecedented Bonding Situation in Viable E (NHB ) (E=Be, Mg; NHB =(HCN ) B) Complexes: Neutral E Forms a Single E-E Covalent Bond. *Angewandte Chemie - International Edition*, **2019**, 58, 8372-8377 | 16.4 | 40 |
| 223 | 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 | 40 |
| 222 | 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 | 2.8 | 40 |
| 221 | Comparative Study on the Noble-Gas Binding Ability of BeX Clusters (X = SO4, CO3, O). *Journal of Physical Chemistry A*, **2015**, 119, 6746-52 | 2.8 | 39 |
| 220 | Selectivity in Gas Adsorption by Molecular Cucurbit[6]uril. *Journal of Physical Chemistry C*, **2016**, 120, 13911-13921 | 3.8 | 35 |
| 219 | Analyzing the efficiency of M n (C2H4) (M = Sc, Ti, Fe, Ni; n = 1, 2) complexes as effective hydrogen storage materials. *Structural Chemistry*, **2011**, 22, 823-837 | 1.8 | 35 |
| 218 | Bonding, Reactivity, and Dynamics in Confined Systems. *Journal of Physical Chemistry A*, **2019**, 123, 4513-4531 | 2.8 | 34 |
| 217 | A coupled-cluster study on the noble gas binding ability of metal cyanides versus metal halides (metal = Cu, Ag, Au). *Journal of Computational Chemistry*, **2015**, 36, 2168-76 | 3.5 | 34 |
| 216 | Structure and stability of (NG)nCN3Be3(+) clusters and comparison with (NG)BeY(0/+). *ChemPhysChem*, **2013**, 14, 2511-7 | 3.2 | 33 |
| 215 | Scrutiny of the HSAB Principle in Some Representative Acid–Base Reactions. *Journal of Physical Chemistry A*, **2001**, 105, 8815-8820 | 2.8 | 32 |
| 214 | Movement of Ng2 molecules confined in a C60 cage: An ab initio molecular dynamics study. *Chemical Physics Letters*, **2014**, 610-611, 351-356 | 2.5 | 31 |
| 213 | A tug-of-war between electronic excitation and confinement in a dynamical context. *Physical Chemistry Chemical Physics*, **2012**, 14, 1716-27 | 3.6 | 31 |
| 212 | Electron Affinity, Electronegativity, and Electrophilicity of Atoms and Ions. *Journal of Chemical & Engineering Data*, **2010**, 55, 1882-1886 | 2.8 | 31 |
| 211 | 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 | 3.6 | 30 |
| 210 | Noble-Noble Strong Union: Gold at Its Best to Make a Bond with a Noble Gas Atom. *ChemistryOpen*, **2019**, 8, 173-187 | 2.3 | 30 |
| 209 | Ab initio study on the stability of Ng(n)BeN, Ng(n)BeN2 and NgBeSiN2 clusters. *ChemPhysChem*, **2014**, 15, 2618-25 | 3.2 | 30 |
| 208 | Density functional theory of chemical hardness **1993**, 11-25 | | 30 |
| 207 | Exploring the nature of silicon-noble gas bonds in H3SiNgNSi and HSiNgNSi compounds (Ng = Xe, Rn). *International Journal of Molecular Sciences*, **2015**, 16, 6402-18 | 6.3 | 29 |

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| 206 | Stability of noble-gas-bound $SiH_4$ clusters. *ChemPhysChem*, **2014**, 15, 3554-64 | 3.2 | 29 |
| 205 | A computational study on the hydrogen adsorption capacity of various lithium-doped boron hydrides. *Journal of Computational Chemistry*, **2012**, 33, 425-34 | 3.5 | 29 |
| 204 | Cucurbiturils as promising hydrogen storage materials: a case study of cucurbit[7]uril. *New Journal of Chemistry*, **2013**, 37, 2492 | 3.6 | 29 |
| 203 | A (T-P) phase diagram of hydrogen storage on (N4C3H)6Li6. *Journal of Physical Chemistry A*, **2012**, 116, 3259-66 | 2.8 | 29 |
| 202 | Synthesis, structure and theoretical studies of Hg(II) NHC carbene complex of annulated ligand pyridinyl[1,2-a]{2-pyridylimidazol}-3-ylidene hexaflurophosphate. *Inorganica Chimica Acta*, **2011**, 375, 271-279 | 2.7 | 29 |
| 201 | Local descriptors around a transition state: a link between chemical bonding and reactivity. *Journal of Physical Chemistry A*, **2005**, 109, 3771-2 | 2.8 | 29 |
| 200 | Noble gas encapsulated B cage. *Physical Chemistry Chemical Physics*, **2018**, 20, 1953-1963 | 3.6 | 29 |
| 199 | How strong are the metallocene-metallocene interactions? Cases of ferrocene, ruthenocene, and osmocene. *Physical Chemistry Chemical Physics*, **2016**, 18, 550-6 | 3.6 | 28 |
| 198 | Synthesis and structure of 1-D Na6 cluster chain with short Na-Na distance: organic like aromaticity in inorganic metal cluster. *Chemical Communications*, **2007**, 135-7 | 5.8 | 28 |
| 197 | Planar pentacoordinate carbon in CGa derivatives. *Physical Chemistry Chemical Physics*, **2018**, 20, 12350-12355 | 3.6 | 27 |
| 196 | Potential use of some metal clusters as hydrogen storage materials--a conceptual DFT approach. *Journal of Molecular Modeling*, **2011**, 17, 777-84 | 2 | 27 |
| 195 | Cyanide-isocyanide isomerization: stability and bonding in noble gas inserted metal cyanides (metal = Cu, Ag, Au). *Physical Chemistry Chemical Physics*, **2018**, 20, 18491-18502 | 3.6 | 26 |
| 194 | Confinement induced binding in noble gas atoms within a BN-doped carbon nanotube. *Chemical Physics Letters*, **2015**, 621, 29-34 | 2.5 | 26 |
| 193 | A possible union of chemical bonding, reactivity, and kinetics. *Journal of Physical Chemistry A*, **2006**, 110, 11401-3 | 2.8 | 26 |
| 192 | Noble gas supported B3+ cluster: formation of strong covalent noble gas–boron bonds. *RSC Advances*, **2016**, 6, 78611-78620 | 3.7 | 26 |
| 191 | Conceptual density functional theory based electronic structure principles. *Chemical Science*, **2021**, 12, 6264-6279 | 9.4 | 26 |
| 190 | Trapping of noble gases (He–Kr) by the aromatic H3+ and Li3+ species: a conceptual DFT approach. *New Journal of Chemistry*, **2010**, 34, 1936 | 3.6 | 25 |
| 189 | Bonding and aromaticity in an all-metal sandwich-like compound, . *Chemical Physics Letters*, **2008**, 460, 382-385 | 2.5 | 25 |

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| 188 | Structure and stability of noble gas bound EX3+ compounds (E = C, Ge, Sn, Pb; X = H, F, Cl, Br). *Journal of Computational Chemistry*, **2016**, 37, 226-36 | 3.5 | 25 |
| 187 | A Spinning Umbrella: Carbon Monoxide and Dinitrogen Bound MB Clusters (M = Co, Rh, Ir). *Journal of Physical Chemistry A*, **2017**, 121, 2971-2979 | 2.8 | 24 |
| 186 | Encapsulation of small gas molecules and rare gas atoms inside the octa acid cavitand. *Theoretical Chemistry Accounts*, **2016**, 135, 1 | 1.9 | 24 |
| 185 | Attractive Xe□i interaction in Li-decorated clusters. *Computational and Theoretical Chemistry*, **2013**, 1021, 62-69 | 2 | 24 |
| 184 | Confinement induced thermodynamic and kinetic facilitation of some Diels-Alder reactions inside a CB[7] cavitand. *Journal of Computational Chemistry*, **2018**, 39, 151-160 | 3.5 | 24 |
| 183 | On the stability of noble gas bound 1-tris(pyrazolyl)borate beryllium and magnesium complexes. *New Journal of Chemistry*, **2015**, 39, 6778-6786 | 3.6 | 23 |
| 182 | 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 | 1.8 | 23 |
| 181 | Finite temperature grand canonical ensemble study of the minimum electrophilicity principle. *Journal of Chemical Physics*, **2017**, 147, 124103 | 3.9 | 23 |
| 180 | Aromaticity in cyclic alkali clusters. *Physical Chemistry Chemical Physics*, **2008**, 10, 2461-74 | 3.6 | 23 |
| 179 | Theoretical study of the trans-N2H2-gis-N2H2 and F2S2-FSSF reactions in gas and solution phases.. *Computational and Theoretical Chemistry*, **2002**, 580, 171-182 | | 23 |
| 178 | MNgCCH (M = Cu, Ag, Au; Ng = Xe, Rn): The First Set of Compounds with M-Ng-C Bonding Motif. *Journal of Physical Chemistry A*, **2017**, 121, 6491-6499 | 2.8 | 22 |
| 177 | Minimum magnetizability principle. *Journal of Chemical Physics*, **2006**, 125, 056101 | 3.9 | 22 |
| 176 | A noble interaction: An assessment of noble gas binding ability of metal oxides (metal = Cu, Ag, Au). *International Journal of Quantum Chemistry*, **2016**, 116, 1016-1024 | 2.1 | 22 |
| 175 | Optical response and gas sequestration properties of metal cluster supported graphene nanoflakes. *Physical Chemistry Chemical Physics*, **2016**, 18, 18811-27 | 3.6 | 21 |
| 174 | Modified Particle Swarm Optimization Algorithms for the Generation of Stable Structures of Carbon Clusters, C ( = 3-6, 10). *Frontiers in Chemistry*, **2019**, 7, 485 | 5 | 21 |
| 173 | Does Confinement Always Lead to Thermodynamically and/or Kinetically Favorable Reactions? A Case Study using Diels-Alder Reactions within ExBox and CB[7]. *ChemPhysChem*, **2017**, 18, 2162-2170 | 3.2 | 20 |
| 172 | Noble Gas Inserted Metal Acetylides (Metal = Cu, Ag, Au). *Journal of Physical Chemistry A*, **2018**, 122, 7391-7401 | 2.7 | 20 |
| 171 | Role of aromaticity and charge of a system in its hydrogen trapping potential and vice versa. *Physical Chemistry Chemical Physics*, **2011**, 13, 20602-14 | 3.6 | 20 |

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| 170 | Two Closely Related Zn(II)-MOFs for Their Large Difference in CO Uptake Capacities and Selective CO Sorption. *Inorganic Chemistry*, **2020**, 59, 7056-7066 | 5.1 | 19 |
| 169 | Pd(II)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 | 2.7 | 19 |
| 168 | Biological Activity and Toxicity: A Conceptual DFT Approach. *Structure and Bonding*, **2013**, 143-179 | 0.9 | 19 |
| 167 | Aromaticity and hydrogen storage capability of planar N64- and N42- rings. *Chemical Physics Letters*, **2011**, 506, 315-320 | 2.5 | 19 |
| 166 | A theoretical investigation on boron-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 | 3.6 | 18 |
| 165 | Reactivity dynamics of a confined molecule in presence of an external magnetic field. *International Journal of Quantum Chemistry*, **2015**, 115, 144-157 | 2.1 | 18 |
| 164 | How Far Can One Push the Noble Gases Towards Bonding?: A Personal Account. *Molecules*, **2019**, 24, | 4.8 | 18 |
| 163 | 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 | 2.8 | 18 |
| 162 | Noble gas encapsulation: clathrate hydrates and their HF doped analogues. *Physical Chemistry Chemical Physics*, **2014**, 16, 17943-54 | 3.6 | 18 |
| 161 | Toward analyzing some neutral and cationic boron–lithium clusters (BxLiy x = 2–6; y = 1, 2) as effective hydrogen storage materials: A conceptual density functional study. *International Journal of Quantum Chemistry*, **2012**, 112, 695-702 | 2.1 | 18 |
| 160 | Stable NCNgNSi (Ng=Kr, Xe, Rn) Compounds with Covalently Bound C-Ng-N Unit: Possible Isomerization of NCNSi through the Release of the Noble Gas Atom. *Chemistry - A European Journal*, **2018**, 24, 2879-2887 | 4.8 | 18 |
| 159 | In quest of a superhalogen supported covalent bond involving a noble gas atom. *Journal of Physical Chemistry A*, **2015**, 119, 3064-74 | 2.8 | 17 |
| 158 | Reactivity dynamics of confined atoms in the presence of an external magnetic field. *European Physical Journal D*, **2014**, 68, 1 | 1.3 | 17 |
| 157 | Bonding, aromaticity, and structure of trigonal dianion metal clusters. *Journal of Computational Chemistry*, **2010**, 31, 1815-21 | 3.5 | 17 |
| 156 | Metal-Organic Frameworks of Cu(II) Constructed from Functionalized Ligands for High Capacity H and CO Gas Adsorption and Catalytic Studies. *Inorganic Chemistry*, **2020**, 59, 1810-1822 | 5.1 | 16 |
| 155 | Noble Gas Binding Ability of Metal-Bipyridine Monocationic Complexes (Metal=Cu, Ag, Au): A Computational Study. *ChemistrySelect*, **2016**, 1, 5842-5849 | 1.8 | 16 |
| 154 | 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 | 16 |
| 153 | A one-pot Garratt–Braverman cyclization and Scholl oxidation route to acene–helicene hybrids. *RSC Advances*, **2013**, 3, 19844 | 3.7 | 16 |

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| 152 | Local hardness equalization and the principle of maximum hardness. *Journal of Chemical Physics*, **2013**, 138, 214103 | 3.9 | 16 |
| 151 | Acidity of meta- and para-substituted aromatic acids: a conceptual DFT study. *New Journal of Chemistry*, **2008**, 32, 1945 | 3.6 | 16 |
| 150 | Exchange□correlation potential and excited-state density functional theory. *International Journal of Quantum Chemistry*, **1996**, 60, 535-543 | 2.1 | 16 |
| 149 | Noble gas bound beryllium chromate and beryllium hydrogen phosphate: a comparison with noble gas bound beryllium oxide. *RSC Advances*, **2016**, 6, 92786-92794 | 3.7 | 15 |
| 148 | Host-guest interactions in ExBox4+. *ChemPhysChem*, **2014**, 15, 4108-16 | 3.2 | 15 |
| 147 | Stability and aromaticity of nH(2)@B(12)N(12) (n=1-12) clusters. *Nano Reviews*, **2011**, 2, | | 15 |
| 146 | Binding of Small Gas Molecules by Metal-Bipyridyl Monocationic Complexes (Metal = Cu, Ag, Au) and Possible Bond Activations Therein. *Journal of Physical Chemistry A*, **2017**, 121, 3803-3817 | 2.8 | 14 |
| 145 | The strongest CO binding and the highest C-O stretching frequency. *Physical Chemistry Chemical Physics*, **2017**, 19, 2286-2293 | 3.6 | 14 |
| 144 | Comment on "Ruling out any electrophilicity equalization principle". *Journal of Physical Chemistry A*, **2012**, 116, 790-1; discussion 792-5 | 2.8 | 14 |
| 143 | Synthesis and structure of a 3D porous network containing aromatic 1D chains of Li(6) rings: experimental and computational studies. *Journal of Physical Chemistry A*, **2010**, 114, 10871-7 | 2.8 | 14 |
| 142 | Substituent effects. *Journal of Physical Chemistry A*, **2005**, 109, 5602-7 | 2.8 | 14 |
| 141 | Boron Nanowheels with Axles Containing Noble Gas Atoms: Viable Noble Gas Bound M□ B Clusters (M=Nb, Ta). *Chemistry - A European Journal*, **2018**, 24, 3590-3598 | 4.8 | 14 |
| 140 | Endohedral gas adsorption by cucurbit[7]uril: a theoretical study. *Physical Chemistry Chemical Physics*, **2017**, 19, 24448-24452 | 3.6 | 13 |
| 139 | Electrophilicity kernel and its hierarchy through softness in conceptual density functional theory. *International Journal of Quantum Chemistry*, **2013**, 113, 2163-2171 | 2.1 | 13 |
| 138 | Aromaticity in all-metal annular systems: the counter-ion effect. *Physical Chemistry Chemical Physics* , **2011**, 13, 14865-78 | 3.6 | 13 |
| 137 | Filling the void: controlled donor-acceptor interaction facilitates the formation of an M-M single bond in the zero oxidation state of M (M = Zn, Cd, Hg). *Dalton Transactions*, **2020**, 49, 1056-1064 | 4.3 | 13 |
| 136 | Structure, stability, and nature of bonding in carbon monoxide bound EX3+ complexes (E = group 14 element; X = H, F, Cl, Br, I). *Journal of Computational Chemistry*, **2016**, 37, 2202-11 | 3.5 | 13 |
| 135 | Stabilization of Boron-Boron Triple Bonds by Mesoionic Carbenes. *ACS Omega*, **2018**, 3, 13720-13730 | 3.9 | 13 |

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| 134 | 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, 23104-11 | 3.6 | 12 |
| 133 | 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 | 9.5 | 12 |
| 132 | Encapsulation of Mg inside a C cage forms an electride. *Journal of Computational Chemistry*, **2020**, 41, 1645-1653 | 3.5 | 12 |
| 131 | Carbo-cages: a computational study. *Journal of Organic Chemistry*, **2014**, 79, 5463-70 | 4.2 | 12 |
| 130 | Catalyst electronic polarizability and enantiomeric excess in asymmetric hydrogenation. *Tetrahedron*, **2010**, 66, 4560-4563 | 2.4 | 12 |
| 129 | A computational study on hydrogenation of CO2, catalyzed by a bridged B/N frustrated Lewis pair. *Structural Chemistry*, **2019**, 30, 1067-1077 | 1.8 | 12 |
| 128 | A Complex Containing Four Magnesium Atoms and Two Mg□Mg Bonds Behaving as an Electride. *European Journal of Inorganic Chemistry*, **2019**, 2019, 4105-4111 | 2.3 | 11 |
| 127 | Redox and Lewis acid-base activities through an electronegativity-hardness landscape diagram. *Journal of Molecular Modeling*, **2013**, 19, 4857-64 | 2 | 11 |
| 126 | Heterotrimetallic compounds containing Mo-M-Li [M = K, Rb and Cs] clusters: synthesis, structure, bonding, aromaticity and theoretical investigations of Li2M2 [M = K and Rb] and Cs4 rings. *Physical Chemistry Chemical Physics*, **2012**, 14, 15579-92 | 3.6 | 11 |
| 125 | Possibility of Having HF-Doped Hydrogen Hydrates. *Journal of Physical Chemistry C*, **2013**, 117, 11625-11634 | 3.3 | 11 |
| 124 | A conceptual density functional study of structure, bonding, reactivity and the possibility of bond-stretch isomerism in some neutral sulfur clusters, S n (n=38). *Journal of Sulfur Chemistry*, **2010**, 31, 231-246 | 2.3 | 11 |
| 123 | Arsenic toxicity: an atom counting and electrophilicity-based protocol. *Molecular Diversity*, **2009**, 13, 551-61 | 3 | 11 |
| 122 | Reactivity Dynamics. *Journal of Physical Chemistry A*, **2021**, 125, 2051-2060 | 2.8 | 11 |
| 121 | HNgBeF3 (Ng = Ar-Rn): Superhalogen-supported noble gas insertion compounds. *International Journal of Quantum Chemistry*, **2018**, 118, e25499 | 2.1 | 11 |
| 120 | Ligand-Supported E Clusters (E=Si-Sn). *Chemistry - A European Journal*, **2017**, 23, 7463-7473 | 4.8 | 10 |
| 119 | NgMCp: Noble Gas Bound Half-Sandwich Complexes (Ng = He-Rn, M = Be-Ba, and Cp = □CH). *Journal of Physical Chemistry A*, **2017**, 121, 3526-3539 | 2.8 | 10 |
| 118 | Cycloaddition Reactions between HC = CHR (R = H, CN, CH) and a Cyclic P/B Frustrated Lewis Pair: A DFT Study. *Journal of Physical Chemistry A*, **2020**, 124, 4455-4462 | 2.8 | 10 |
| 117 | Fixation of nitrous oxide (N2O) by 1, 4, 2, 5-diazadiborinine: A DFT study. *International Journal of Quantum Chemistry*, **2018**, 118, e25593 | 2.1 | 10 |

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| 29 | Box-Shaped Hosts: Evaluation of the Interaction Nature and Host Characteristics of ExBox Derivatives in Host-Guest Complexes from Computational Methods **2021**, 395-416 | | 1 |
| 28 | Unveiling the Mysterious Mechanisms of Chemical Reactions **2021**, 81-97 | | 1 |
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| 26 | Effect of confinement on the behavior of superhalogen and superalkali. *Computational and Theoretical Chemistry*, **2021**, 1206, 113491 | 2 | 0 |
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# List of Publications

8 Conceptual density functional theory and aromaticity **2021**, 285-319

7 Hydrogen Storage in All-Metal and Nonmetal Aromatic Clusters **2018**, 329-362

6 Pressure-Induced Phase Transitions **2021**, 25-47

5 Confinement Induced Chemical Bonding: Case of Noble Gases **2021**, 239-261

4 A Perspective on the So-Called Dual Descriptor **2021**, 99-112

3 Effect of Confinement on Gas Storage Potential and Catalytic Activity **2021**, 273-291

2 Chemical Reactivity in Time-Dependent Situations **2022**, 161-185

1 Possible catalytic activity of N,N-coordinated mono-cationic copper bound Pyrazol-1-yl(1H-pyrrol-2-yl)methanone complex: a computational study. *Proceedings of the Indian National Science Academy*,1 1