# 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 |
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| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Fischer and Schrock carbene complexes in the light of global and local electrophilicityâ€based descriptors. Journal of Physical Organic Chemistry, 2023, 36, . | 1.9 | 2 |
| 2 | Variation in electrophilicity on electronic excitation. Journal of Physical Organic Chemistry, 2023, 36, . | 1.9 | 9 |
| 3 | Electrophilicity index revisited. Journal of Computational Chemistry, 2023, 44, 278-297. | 3.3 | 28 |
| 4 | Possible C-F bond activation by B(C6F5)3/lutidine and Al(C6F5)3/lutidine frustrated Lewis pair: an in silico study. Journal of Chemical Sciences, 2022, 134, 1. | 1.5 | 9 |
| 5 | Stabilisation of Li(0)-Li(0) bond by normal and mesoionic carbenes and electride characteristics of the complexes. Molecular Physics, 2022, 120, . | 1.7 | 4 |
| 6 | Activation of Small Molecules and Hydrogenation of CO2 Catalyzed by Frustrated Lewis Pairs. Catalysts, 2022, 12, 201. | 3.5 | 19 |
| 7 | <scp>CSiGaAl<sub>2</sub></scp><sup>â^'/0</sup>and<scp>CGeGaAl<sub>2</sub></scp><sup>â^'/0</sup>having planar tetracoordinate carbon atoms in their global minimum energy structures. Journal of Computational Chemistry, 2022, 43, 894-905. | 3.3 | 14 |
| 8 | <scp>Li<sub>4</sub>EPc</scp>: A metalloâ€organic electride comprising metalâ€nitrogen bonds. International Journal of Quantum Chemistry, 2022, 122, . | 2.0 | 2 |
| 9 | Revisiting the trapping of noble gases (Heâ€“Kr) by the triatomic H3+ and Li3+ species: a density functional reactivity theory study. Journal of Molecular Modeling, 2022, 28, 122. | 1.8 | 2 |
| 10 | Small molecule activation and dehydrogenation of an amineâ€“borane system using frustrated Lewis pairs. Structural Chemistry, 2022, 33, 1853-1865. | 2.0 | 9 |
| 11 | Controlling Tunneling Oscillation and Quantum Localization in an Asymmetric Double-Well Potential: A Bohmian Perspective. Journal of Physical Chemistry A, 2022, 126, 4834-4847. | 2.5 | 1 |
| 12 | Can superalkalis and superhalogens improve the efficacy of redox reactions?. Chemical Physics Letters, 2021, 762, 138131. | 2.6 | 2 |
| 13 | Density functional theory studies of boron clusters with exotic properties in bonding, aromaticity and reactivity. Physical Chemistry Chemical Physics, 2021, 23, 24118-24124. | 2.8 | 11 |
| 14 | Conceptual density functional theory and aromaticity. , 2021, , 285-319. | | 1 |
| 15 | Chemical reactivity from a conceptual density functional theory perspective. Journal of the Indian Chemical Society, 2021, 98, 100008. | 2.8 | 15 |
| 16 | Possible effects of fluxionality of a cavitand on its catalytic activity through confinement. Physical Chemistry Chemical Physics, 2021, 23, 15817-15834. | 2.8 | 5 |
| 17 | Reactivity Dynamics. Journal of Physical Chemistry A, 2021, 125, 2051-2060. | 2.5 | 34 |
| 18 | Editorial: â€œChanging the Perspective of the Noble Gas Reactivityâ€. Frontiers in Chemistry, 2021, 9, 658318. | 3.6 | 1 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | Comparison Between Electride Characteristics of Li3@B40 and Li3@C60. Frontiers in Chemistry, 2021, 9, 638581. | 3.6 | 11 |
| 20 | Determination of stable structure of a cluster using convolutional neural network and particle swarm optimization. Theoretical Chemistry Accounts, 2021, 140, 1. | 1.4 | 14 |
| 21 | Does confinement alter the ionization energy and electron affinity of atoms?. European Physical Journal D, 2021, 75, 1. | 1.3 | 5 |
| 22 | Electride characteristics of M2(Î·5-E5)2 (M = Be, Mg; E = Sb5-). Structural Chemistry, 2021, 32, 2107-2114. | 2.0 | 5 |
| 23 | H2 adsorption by noble gas insertion compounds: A computational study. Journal of the Indian Chemical Society, 2021, 98, 100060. | 2.8 | 1 |
| 24 | Local Temperature as a Chemical Reactivity Descriptor. Journal of Physical Chemistry Letters, 2021, 12, 5623-5630. | 4.6 | 17 |
| 25 | Substituent Effects on Electride Characteristics of Mg<sub>2</sub>(Î·<sup>5</sup>-C<sub>5</sub>H<sub>5</sub>)<sub>2</sub>: A Theoretical Study. Journal of Physical Chemistry A, 2021, 125, 6207-6220. | 2.5 | 10 |
| 26 | Biological Activity, Physical Properties, and Toxicity. International Journal of Quantitative Structure-Property Relationships, 2021, 6, 25-34. | 0.5 | 1 |
| 27 | Conceptual DFT based electronic structure principles in a dynamical context. Journal of the Indian Chemical Society, 2021, 98, 100098. | 2.8 | 10 |
| 28 | A computational investigation of the activation of allene (H2CÂ=ÂCÂ=ÂCHR; RÂ=ÂH, CH3, CN) by a frustrated phosphorous/boron Lewis pair. Chemical Physics Letters, 2021, 774, 138623. | 2.6 | 14 |
| 29 | Atomic Clusters: Structure, Reactivity, Bonding, and Dynamics. Frontiers in Chemistry, 2021, 9, 730548. | 3.6 | 14 |
| 30 | In Silico Studies on Selected Neutral Molecules, CGa2Ge2, CAlGaGe2, and CSiGa2Ge Containing Planar Tetracoordinate Carbon. Atoms, 2021, 9, 65. | 1.6 | 16 |
| 31 | Conceptual density functional theory based electronic structure principles. Chemical Science, 2021, 12, 6264-6279. | 7.4 | 96 |
| 32 | Self-healable functional polymers based on Dielsâ€“Alder â€˜click chemistryâ€™ involving substituted furan and triazolinedione derivatives: a simple and very fast approach. Polymer Chemistry, 2021, 12, 6283-6290. | 3.9 | 4 |
| 33 | Effect of confinement on the behavior of superhalogen and superalkali. Computational and Theoretical Chemistry, 2021, 1206, 113491. | 2.5 | 2 |
| 34 | Aromatic Clusters as Potential Hydrogen Storage Materials. Frontiers in Energy Research, 2021, 9, . | 2.3 | 3 |
| 35 | XNgNSi (X = HCC, F; Ng = Kr, Xe, Rn): A New Class of Metastable Insertion Compounds Containing Ngâ€“C/F and Ngâ€“N Bonds and Possible Isomerization therein. Journal of Physical Chemistry A, 2021, , . | 2.5 | 2 |
| 36 | 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 |

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| 37 | 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 |
| 38 | Ligand stabilized transient â€œMNCâ€•and its influence on MNCâ€‰â†’â€‰MCN isomerization process: a computational study (Mâ€‰=â€‰Cu, Ag, and Au). Theoretical Chemistry Accounts, 2020, 139, 1. | 1.4 | 3 |
| 39 | Towards understanding metal aromaticity in different spin states: A density functional theory and information-theoretic approach analysis. Chemical Physics Letters, 2020, 761, 138065. | 2.6 | 13 |
| 40 | Electride Characteristics of Some Binuclear Sandwich Complexes of Alkaline Earth Metals, M<sub>2</sub>(Î·<sup>5</sup>-L)<sub>2</sub>(M = Be, Mg; L =) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 622 Td (C<sub>5</sub>H<sub | 2.5 | 17 |
| 41 | Can a decrease in anti-aromaticity increase the dihydrogen activation ability of a frustrated phosphorous/borane Lewis pair?: a DFT study. Theoretical Chemistry Accounts, 2020, 139, 1. | 1.4 | 10 |
| 42 | Changes in Structure and Reactivity of Ng2 Encapsulated in Fullerenes: A Density Functional Theory Study. Frontiers in Chemistry, 2020, 8, 566. | 3.6 | 7 |
| 43 | Noble Gas Binding Ability of an Au(I) Cation Stabilized by a Frustrated Lewis Pair: A DFT Study. Frontiers in Chemistry, 2020, 8, 616. | 3.6 | 4 |
| 44 | Intriguing structural, bonding and reactivity features in some beryllium containing complexes. Physical Chemistry Chemical Physics, 2020, 22, 27476-27495. | 2.8 | 10 |
| 45 | Fast â€œES-Clickâ€•Reaction Involving Furfuryl and Triazolinedione Functionalities toward Designing a Healable Polymethacrylate. Macromolecules, 2020, 53, 8313-8323. | 4.8 | 11 |
| 46 | Effect of substitution on the bonding in He dimer confined within dodecahedrane: A computational study. Journal of Computational Chemistry, 2020, 41, 2398-2405. | 3.3 | 5 |
| 47 | Cycloaddition Reactions between H<sub>2</sub>C = CHR (R = H, CN, CH<sub>3</sub>) and a Cyclic P/B Frustrated Lewis Pair: A DFT Study. Journal of Physical Chemistry A, 2020, 124, 4455-4462. | 2.5 | 18 |
| 48 | 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 |
| 49 | Tribute to Paul Geerlings. Journal of Physical Chemistry A, 2020, 124, 5061-5062. | 2.5 | 0 |
| 50 | Integrating firefly algorithm with density functional theory for global optimization of Al42â^' clusters. Theoretical Chemistry Accounts, 2020, 139, 1. | 1.4 | 7 |
| 51 | 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 |
| 52 | Conceptual density functional theory: status, prospects, issues. Theoretical Chemistry Accounts, 2020, 139, 1. | 1.4 | 249 |
| 53 | Metalâ€“Organic Frameworks of Cu(II) Constructed from Functionalized Ligands for High Capacity H<sub>2</sub> and CO<sub>2</sub> Gas Adsorption and Catalytic Studies. Inorganic Chemistry, 2020, 59, 1810-1822. | 4.0 | 25 |
| 54 | Encapsulation of Mg<sub>2</sub> inside a C<sub>60</sub> cage forms an electride. Journal of Computational Chemistry, 2020, 41, 1645-1653. | 3.3 | 20 |

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| 55 | Two Closely Related Zn(II)-MOFs for Their Large Difference in CO<sub>2</sub> Uptake Capacities and Selective CO<sub>2</sub> Sorption. Inorganic Chemistry, 2020, 59, 7056-7066. | 4.0 | 35 |
| 56 | A conceptual DFT analysis of the plausible mechanism of some pericyclic reactions. Structural Chemistry, 2020, 31, 1745-1756. | 2.0 | 8 |
| 57 | Quantitative Structure-Toxicity Relationship Models Based on Hydrophobicity and Electrophilicity. Methods in Pharmacology and Toxicology, 2020, , 661-679. | 0.2 | 5 |
| 58 | How Far Can One Push the Noble Gases Towards Bonding?: A Personal Account. Molecules, 2019, 24, 2933. | 3.8 | 34 |
| 59 | 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 |
| 60 | 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 |
| 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 | 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 |
| 63 | 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 |
| 64 | 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 |
| 65 | Microsolvation of lithiumâ€“phosphorus double helix: a DFT study. Theoretical Chemistry Accounts, 2019, 138, 1. | 1.4 | 2 |
| 66 | Bonding, Reactivity, and Dynamics in Confined Systems. Journal of Physical Chemistry A, 2019, 123, 4513-4531. | 2.5 | 48 |
| 67 | Unprecedented Bonding Situation in Viable E<sub>2</sub>(NHB<sup>Me</sup>)<sub>2</sub> (E=Be,) Tj ETQq1 1 0.784314 rgBT /O<br>Forms a Single Eâˆ’E Covalent Bond. Angewandte Chemie, 2019, 131, 8460-8465. | 2.0 | 22 |
| 68 | Unprecedented Bonding Situation in Viable E<sub>2</sub>(NHB<sup>Me</sup>)<sub>2</sub> (E=Be,) Tj ETQq0 0 0 rgBT /Overlock 10<br>Forms a Single Eâˆ’E Covalent Bond. Angewandte Chemie - International Edition, 2019, 58, 8372-8377. | 13.8 | 62 |
| 69 | An Intramolecular Charge Transfer Induced Fluorescent Chemosensor for Selective Detection of Mercury (II) and its Selfâ€Turnâ€On Inside Live Cells at Physiological pH. ChemistrySelect, 2019, 4, 4810-4819. | 1.5 | 11 |
| 70 | An In Silico QSAR Model Study Using Electrophilicity as a Possible Descriptor Against T. Brucei. International Journal of Chemoinformatics and Chemical Engineering, 2019, 8, 57-68. | 0.1 | 3 |
| 71 | A comparative study to predict regioselectivity, electrophilicity and nucleophilicity with Fukui function and Hirshfeld charge. Theoretical Chemistry Accounts, 2019, 138, 1. | 1.4 | 138 |
| 72 | Donorâ€“Acceptor vs Electron-Shared Bonding: Triatomic Si<sub>n</sub>C<sub>3â€“n</sub> (n â‰¤ 3) Clusters Stabilized by Cyclic Alkyl(amino) Carbene. Journal of Physical Chemistry A, 2019, 123, 10764-10771. | 2.5 | 5 |

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| 73 | Hydrophobicity versus electrophilicity: A new protocol toward quantitative structureâ€“toxicity relationship. Chemical Biology and Drug Design, 2019, 93, 1083-1095. | 3.2 | 18 |
| 74 | 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 |
| 75 | Frontispiece: 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, . | 3.3 | 0 |
| 76 | Fixation of nitrous oxide (N<sub>2</sub>O) by 1, 4, 2, 5â€diazadiborinine: A DFT study. International Journal of Quantum Chemistry, 2018, 118, e25593. | 2.0 | 14 |
| 77 | Diagrams for comprehensive molecular orbital-based chemical reaction analyses: reactive orbital energy diagrams. Physical Chemistry Chemical Physics, 2018, 20, 14211-14222. | 2.8 | 8 |
| 78 | Planar pentacoordinate carbon in CGa<sub>5</sub><sup>+</sup> derivatives. Physical Chemistry Chemical Physics, 2018, 20, 12350-12355. | 2.8 | 41 |
| 79 | Tunneling and quantum localization in chaosâ€driven symmetric triple well potential: An approach using quantum theory of motion. International Journal of Quantum Chemistry, 2018, 118, e25531. | 2.0 | 3 |
| 80 | Reactions involving some gas molecules through sequestration on Al<sub>12</sub>Be cluster: An electron density based study. Journal of Computational Chemistry, 2018, 39, 535-545. | 3.3 | 5 |
| 81 | Hostâ€“guest interactions between octa acid and cations/nucleobases. Journal of Computational Chemistry, 2018, 39, 161-175. | 3.3 | 12 |
| 82 | 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 |
| 83 | Boron Nanowheels with Axles Containing Noble Gas Atoms: Viable Noble Gas Bound MÂ©B<sub>10</sub><sup>â^'</sup> Clusters (M=Nb, Ta). Chemistry - A European Journal, 2018, 24, 3590-3598. | 3.3 | 19 |
| 84 | Noble gas encapsulated B<sub>40</sub> cage. Physical Chemistry Chemical Physics, 2018, 20, 1953-1963. | 2.8 | 41 |
| 85 | A possible reason behind the initial formation of pentagonal dodecahedron cavities in sI-methane hydrate nucleation: A DFT study. Chemical Physics Letters, 2018, 691, 415-420. | 2.6 | 3 |
| 86 | 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 |
| 87 | HNgBeF<sub>3</sub> (Ngâ€‰=â€‰Arâ€Rn): Superhalogenâ€supported noble gas insertion compounds. International Journal of Quantum Chemistry, 2018, 118, e25499. | 2.0 | 15 |
| 88 | Hydrogen Storage in All-Metal and Nonmetal Aromatic Clusters. , 2018, , 329-362. | | 0 |
| 89 | Adsorption of Molecular Hydrogen on Lithiumâ€“Phosphorus Double-Helices. Journal of Physical Chemistry C, 2018, 122, 27941-27946. | 3.1 | 7 |
| 90 | Activation of Small Molecules (H<sub>2</sub>, CO<sub>2</sub>, N<sub>2</sub>O, CH<sub>4</sub>,) Tj ETQq0 0 0 rgBT /Overlock 1<br>Omega, 2018, 3, 17199-17211. | 3.5 | 13 |

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| 91 | Stabilization of Boronâ€“Boron Triple Bonds by Mesoionic Carbenes. ACS Omega, 2018, 3, 13720-13730. | 3.5 | 17 |
| 92 | Analyzing torquoselectivity in a series of unusual ringâ€opening reactions through bond reactivity indices and the adaptive natural density partitioning method. International Journal of Quantum Chemistry, 2018, 118, e25778. | 2.0 | 5 |
| 93 | A (Tâ€“P) phase diagram for the adsorption/desorption of carbon dioxide and hydrogen in a Cu(II)-MOF. Polyhedron, 2018, 153, 254-260. | 2.2 | 7 |
| 94 | Exohedral complexation of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" overflow="scroll"><mml:mrow><mml:msubsup><mml:mi mathvariant="normal">B</mml:mi><mml:mrow><mml:mn>39</mml:mn></mml:mrow><mml:mo>-</mml:mo></mml:msubsup></mml:r with ECpâ^—+ half-sandwich complexes (E Si, Ge, Sn, Pb): A DFT study. Computational and Theoretical Chemistry, 2018, 1140, 49-55. | 2.8 | 1 |
| 95 | Noble Gas Inserted Metal Acetylides (Metal = Cu, Ag, Au). Journal of Physical Chemistry A, 2018, 122, 7391-7401. | 2.5 | 25 |
| 96 | A machine learning technique toward generating minimum energy structures of small boron clusters. International Journal of Quantum Chemistry, 2018, 118, e25672. | 2.0 | 11 |
| 97 | Confinement induced catalytic activity in a Diels-Alder reaction: comparison among various CB[n], nâ€‰=â€‰6â€“8, cavitands. Journal of Molecular Modeling, 2018, 24, 228. | 1.8 | 7 |
| 98 | Cyanideâ€“isocyanide isomerization: stability and bonding in noble gas inserted metal cyanides (metal =) Tj ETQq0 0 0 rgBT /Overlock 1 | 2.8 | 32 |
| 99 | Aromaticity in the Light of Magnetic Criteria. Current Organic Chemistry, 2018, 21, . | 1.6 | 0 |
| 100 | Ligandâ€Supported E<sub>3</sub> Clusters (E=Siâ€“Sn). Chemistry - A European Journal, 2017, 23, 7463-7473. | 3.3 | 11 |
| 101 | NgMCp<sup>+</sup>: Noble Gas Bound Half-Sandwich Complexes (Ng = Heâ€“Rn, M = Beâ€“Ba, and Cp =) Tj ETQq1 1 0.784314 rgBT | 2.5 | 13 |
| 102 | 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 |
| 103 | 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 |
| 104 | Does Confinement Always Lead to Thermodynamically and/or Kinetically Favorable Reactions? A Case Study using Dielsâ€“Alder Reactions within ExBox<sup>+4</sup> and CB[7]. ChemPhysChem, 2017, 18, 2162-2170. | 2.1 | 24 |
| 105 | Frontispiece: Ligandâ€Supported E<sub>3</sub> Clusters (E=Siâ€“Sn). Chemistry - A European Journal, 2017, 23, . | 3.3 | 0 |
| 106 | Modeling of 1-D Nanowires and analyzing their Hydrogen and Noble Gas Binding Ability. Journal of Chemical Sciences, 2017, 129, 849-858. | 1.5 | 10 |
| 107 | A Spinning Umbrella: Carbon Monoxide and Dinitrogen Bound MB<sub>12</sub><sup>â€“</sup> Clusters (M = Co, Rh, Ir). Journal of Physical Chemistry A, 2017, 121, 2971-2979. | 2.5 | 31 |
| 108 | The strongest CO binding and the highest Câ€“O stretching frequency. Physical Chemistry Chemical Physics, 2017, 19, 2286-2293. | 2.8 | 19 |

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| 109 | Effect of functionalization of boron nitride flakes by main group metal clusters on their optoelectronic properties. Journal of Physics Condensed Matter, 2017, 29, 425201. | 1.8 | 6 |
| 110 | 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 |
| 111 | Change in optoelectronic properties of ExBox<sup>+4</sup> on functionalization and guest encapsulation. Physical Chemistry Chemical Physics, 2017, 19, 23373-23385. | 2.8 | 10 |
| 112 | Endohedral gas adsorption by cucurbit[7]uril: a theoretical study. Physical Chemistry Chemical Physics, 2017, 19, 24448-24452. | 2.8 | 13 |
| 113 | Does Confinement Always Lead to Thermodynamically and/or Kinetically Favorable Reactions? A Case Study using Diels-Alder Reactions within ExBox+4 and CB[7]. ChemPhysChem, 2017, 18, 2136-2136. | 2.1 | 0 |
| 114 | Finite temperature grand canonical ensemble study of the minimum electrophilicity principle. Journal of Chemical Physics, 2017, 147, 124103. | 3.0 | 33 |
| 115 | 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 |
| 116 | Role of Lithium Decoration on Hydrogen Storage Potential. Journal of the Mexican Chemical Society, 2017, 56, . | 0.6 | 4 |
| 117 | Quantitative Structure-Activity/Property/Toxicity Relationships through Conceptual Density Functional Theory-Based Reactivity Descriptors. , 2017, , 1517-1572. | | 7 |
| 118 | Favorable Direction in a Chemical Reaction Through the Maximum Hardness Principle. Journal of the Mexican Chemical Society, 2017, 57, . | 0.6 | 0 |
| 119 | Statistical Significance of the Maximum Hardness Principle Applied to Some Selected Chemical Reactions. Molecules, 2016, 21, 1477. | 3.8 | 7 |
| 120 | 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 |
| 121 | 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 |
| 122 | Solution of the â€œClassicalâ€•SchrÃ¶dinger equation for a driven symmetric triple well: A comparison with its classical counterpart. International Journal of Quantum Chemistry, 2016, 116, 1224-1243. | 2.0 | 8 |
| 123 | Possible sequestration of polar gas molecules by superhalogen supported aluminum nitride nanoflakes. Journal of Molecular Modeling, 2016, 22, 271. | 1.8 | 3 |
| 124 | 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 |
| 125 | Structure, stability, and nature of bonding in carbon monoxide bound complexes (Eâ€‰=â€‰group 14 element;) Tj ETQq1 1 0.784314 | 3.3 | 13 |
| 126 | Noble gas supported B<sub>3</sub><sup>+</sup> cluster: formation of strong covalent noble gasâ€“boron bonds. RSC Advances, 2016, 6, 78611-78620. | 3.6 | 40 |

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| 127 | 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 |
| 128 | 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 |
| 129 | Sequestration and Activation of Small Gas Molecules on BN-Flakes and the Effect of Various Metal Oxide Molecules therein. Journal of Physical Chemistry C, 2016, 120, 27782-27799. | 3.1 | 9 |
| 130 | Noble Gas Binding Ability of Metalâ€Bipyridine Monocationic Complexes (Metal=Cu, Ag, Au): A Computational Study. ChemistrySelect, 2016, 1, 5842-5849. | 1.5 | 18 |
| 131 | Encapsulation of small gas molecules and rare gas atoms inside the octa acid cavitand. Theoretical Chemistry Accounts, 2016, 135, 1. | 1.4 | 29 |
| 132 | Optical response and gas sequestration properties of metal cluster supported graphene nanoflakes. Physical Chemistry Chemical Physics, 2016, 18, 18811-18827. | 2.8 | 26 |
| 133 | Selectivity in Gas Adsorption by Molecular Cucurbit[6]uril. Journal of Physical Chemistry C, 2016, 120, 13911-13921. | 3.1 | 49 |
| 134 | How strong are the metalloceneâ€“metallocene interactions? Cases of ferrocene, ruthenocene, and osmocene. Physical Chemistry Chemical Physics, 2016, 18, 550-556. | 2.8 | 34 |
| 135 | Structure and bonding of IrB<sub>12</sub><sup>â^'</sup>: converting a rigid boron B<sub>12</sub> platelet to a Wankel motor. RSC Advances, 2016, 6, 27177-27182. | 3.6 | 67 |
| 136 | Viability of aromatic all-pnictogen anions. Physical Chemistry Chemical Physics, 2016, 18, 11738-11745. | 2.8 | 9 |
| 137 | Ïƒ-Aromatic cyclic M<sub>3</sub><sup>+</sup> (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 |
| 138 | Dynamical behavior of Borospherene: A Nanobubble. Scientific Reports, 2015, 5, 11287. | 3.3 | 81 |
| 139 | Fermi accelerator: A new insight from quantum theory of motion. International Journal of Quantum Chemistry, 2015, 115, 1733-1738. | 2.0 | 4 |
| 140 | Three-dimensional networks containing rectangular Sr4and Ba4units: Synthesis, structure, bonding, and potential application for Ne gas separation. International Journal of Quantum Chemistry, 2015, 115, 1501-1510. | 2.0 | 6 |
| 141 | Comparative Study on the Noble-Gas Binding Ability of BeX Clusters (X = SO<sub>4</sub>,) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf | 2.5 | 47 |
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