Pratim Kumar Chattaraj

List of Publications by Year in Descending Order

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	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	1.8	2
276	Activation of Small Molecules and Hydrogenation of CO2 Catalyzed by Frustrated Lewis Pairs. *Catalysts*, **2022**, 12, 201	4	1
275	CSiGaAl and CGeGaAl having planar tetracoordinate carbon atoms in their global minimum energy structures.. *Journal of Computational Chemistry*, **2022**,	3.5	4
274	Revisiting the trapping of noble gases (He-Kr) by the triatomic H and Li species: a density functional reactivity theory study.. *Journal of Molecular Modeling*, **2022**, 28, 122	2	0
273	Chemical Reactivity in Time-Dependent Situations **2022**, 161-185		
272	A Conceptual DFT Approach Toward Analyzing Hydrogen Storage Potential **2022**, 533-553		0
271	Effect of confinement on the behavior of superhalogen and superalkali. *Computational and Theoretical Chemistry*, **2021**, 1206, 113491	2	0
270	Comparison Between Electride Characteristics of Li@B and Li@C. *Frontiers in Chemistry*, **2021**, 9, 6385815		6
269	Determination of stable structure of a cluster using convolutional neural network and particle swarm optimization. *Theoretical Chemistry Accounts*, **2021**, 140, 1	1.9	7
268	Does confinement alter the ionization energy and electron affinity of atoms?. *European Physical Journal D*, **2021**, 75, 1	1.3	2
267	Electride characteristics of M2(□-E5)2 (M = Be, Mg; E = Sb5-). *Structural Chemistry*, **2021**, 32, 2107	1.8	1
266	H2 adsorption by noble gas insertion compounds: A computational study. *Journal of the Indian Chemical Society*, **2021**, 98, 100060		1
265	Local Temperature as a Chemical Reactivity Descriptor. *Journal of Physical Chemistry Letters*, **2021**, 12, 5623-5630	6.4	7
264	Substituent Effects on Electride Characteristics of Mg(□CH): A Theoretical Study. *Journal of Physical Chemistry A*, **2021**, 125, 6207-6220	2.8	4
263	Biological Activity, Physical Properties, and Toxicity. *International Journal of Quantitative Structure-Property Relationships*, **2021**, 6, 25-34	1.2	0
262	Conceptual DFT based electronic structure principles in a dynamical context. *Journal of the Indian Chemical Society*, **2021**, 98, 100098		0
261	A computational investigation of the activation of allene (H2C = C = CHR; R = H, CH3, CN) by a frustrated phosphorous/boron Lewis pair. *Chemical Physics Letters*, **2021**, 774, 138623	2.5	4

260	Can superalkalis and superhalogens improve the efficacy of redox reactions?. *Chemical Physics Letters*, **2021**, 762, 138131	2.5	2
259	Density functional theory studies of boron clusters with exotic properties in bonding, aromaticity and reactivity. *Physical Chemistry Chemical Physics*, **2021**, 23, 24118-24124	3.6	2
258	Conceptual density functional theory and aromaticity **2021**, 285-319		
257	Chemical reactivity from a conceptual density functional theory perspective. *Journal of the Indian Chemical Society*, **2021**, 98, 100008		3
256	Possible effects of fluxionality of a cavitand on its catalytic activity through confinement. *Physical Chemistry Chemical Physics*, **2021**, 23, 15817-15834	3.6	3
255	Reactivity Dynamics. *Journal of Physical Chemistry A*, **2021**, 125, 2051-2060	2.8	11
254	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
253	Pressure-Induced Phase Transitions **2021**, 25-47		
252	Atomic Clusters: Structure, Reactivity, Bonding, and Dynamics. *Frontiers in Chemistry*, **2021**, 9, 730548	5	4
251	Conceptual DFT and Confinement **2021**, 49-67		0
250	Engineering the Confined Space of MOFs for Heterogeneous Catalysis of Organic Transformations **2021**, 293-333		2
249	Confinement Induced Chemical Bonding: Case of Noble Gases **2021**, 239-261		
248	Chemical Binding and Reactivity Parameters: A Unified Coarse Grained Density Functional View **2021**, 167-177		0
247	Unveiling the Mysterious Mechanisms of Chemical Reactions **2021**, 81-97		1
246	A Perspective on the So-Called Dual Descriptor **2021**, 99-112		
245	Conceptual Density Functional Theory in the Grand Canonical Ensemble **2021**, 191-211		1
244	Effect of Confinement on Gas Storage Potential and Catalytic Activity **2021**, 273-291		
243	Chemical Reactivity Within the Spin-Polarized Framework of Density Functional Theory **2021**, 135-165		0

242	In Silico Studies on Selected Neutral Molecules, CGa2Ge2, CAlGaGe2, and CSiGa2Ge Containing Planar Tetracoordinate Carbon. *Atoms*, **2021**, 9, 65	2.1	5
241	Conceptual density functional theory based electronic structure principles. *Chemical Science*, **2021**, 12, 6264-6279	9.4	26
240	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
239	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
238	Tribute to Paul Geerlings. *Journal of Physical Chemistry A*, **2020**, 124, 5061-5062	2.8	
237	Integrating firefly algorithm with density functional theory for global optimization of Al42 clusters. *Theoretical Chemistry Accounts*, **2020**, 139, 1	1.9	7
236	Flexibility Induced Encapsulation of Ultrafine Palladium Nanoparticles into Organic Cages for Tsuji-Trost Allylation. *ACS Applied Materials & Interfaces*, **2020**, 12, 8539-8546	9.5	9
235	Conceptual density functional theory: status, prospects, issues. *Theoretical Chemistry Accounts*, **2020**, 139, 1	1.9	113
234	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
233	Encapsulation of Mg inside a C cage forms an electride. *Journal of Computational Chemistry*, **2020**, 41, 1645-1653	3.5	12
232	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
231	Quantitative structure-toxicity relationship: An in silico study using electrophilicity and hydrophobicity as descriptors. *International Journal of Quantum Chemistry*, **2020**, 120, e26097	2.1	7
230	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
229	Ligand stabilized transient MNC and its influence on MNC -gMCN isomerization process: a computational study (M = Cu, Ag, and Au). *Theoretical Chemistry Accounts*, **2020**, 139, 1	1.9	1
228	Towards understanding metal aromaticity in different spin states: A density functional theory and information-theoretic approach analysis. *Chemical Physics Letters*, **2020**, 761, 138065	2.5	6
227	Electride Characteristics of Some Binuclear Sandwich Complexes of Alkaline Earth Metals, M(L) (M = Be, Mg; L = CH, N, P, As). *Journal of Physical Chemistry A*, **2020**, 124, 9801-9810	2.8	9
226	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	1.9	5
225	Changes in Structure and Reactivity of Ng Encapsulated in Fullerenes: A Density Functional Theory Study. *Frontiers in Chemistry*, **2020**, 8, 566	5	3

224	Noble Gas Binding Ability of an Au(I) Cation Stabilized by a Frustrated Lewis Pair: A DFT Study. *Frontiers in Chemistry*, **2020**, 8, 616	5	0
223	Intriguing structural, bonding and reactivity features in some beryllium containing complexes. *Physical Chemistry Chemical Physics*, **2020**, 22, 27476-27495	3.6	2
222	Fast Thiol-Click Reaction Involving Furfuryl and Triazolinedione Functionalities toward Designing a Healable Polymethacrylate. *Macromolecules*, **2020**, 53, 8313-8323	5.5	5
221	Effect of substitution on the bonding in He dimer confined within dodecahedrane: A computational study. *Journal of Computational Chemistry*, **2020**, 41, 2398-2405	3.5	4
220	A conceptual DFT analysis of the plausible mechanism of some pericyclic reactions. *Structural Chemistry*, **2020**, 31, 1745-1756	1.8	3
219	Quantitative Structure-Toxicity Relationship Models Based on Hydrophobicity and Electrophilicity. *Methods in Pharmacology and Toxicology*, **2020**, 661-679	1.1	3
218	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
217	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
216	Microsolvation of lithium–phosphorus double helix: a DFT study. *Theoretical Chemistry Accounts*, **2019**, 138, 1	1.9	1
215	Bonding, Reactivity, and Dynamics in Confined Systems. *Journal of Physical Chemistry A*, **2019**, 123, 4513-4831	2.8	34
214	Unprecedented Bonding Situation in Viable E2(NHBMe)2 (E=Be, Mg; NHBMe=(HCNMe)2B) Complexes: Neutral E2 Forms a Single E–E Covalent Bond. *Angewandte Chemie*, **2019**, 131, 8460	3.6	
213	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
212	An Intramolecular Charge Transfer Induced Fluorescent Chemosensor for Selective Detection of Mercury (II) and its Self-Turn-On Inside Live Cells at Physiological pH. *ChemistrySelect*, **2019**, 4, 4810-4819	1.8	8
211	How Far Can One Push the Noble Gases Towards Bonding?: A Personal Account. *Molecules*, **2019**, 24,	4.8	18
210	A new healable polymer material based on ultrafast Diels–Alder 'click' chemistry using triazolinedione and fluorescent anthracyl derivatives: a mechanistic approach. *Polymer Chemistry*, **2019**, 10, 5070-5079	4.9	7
209	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
208	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
207	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

206	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	0.3	0
205	A comparative study to predict regioselectivity, electrophilicity and nucleophilicity with Fukui function and Hirshfeld charge. *Theoretical Chemistry Accounts*, **2019**, 138, 1	1.9	50
204	Donor-Acceptor vs Electron-Shared Bonding: Triatomic SiC (B) Clusters Stabilized by Cyclic Alkyl(amino) Carbene. *Journal of Physical Chemistry A*, **2019**, 123, 10764-10771	2.8	3
203	Hydrophobicity versus electrophilicity: A new protocol toward quantitative structure-toxicity relationship. *Chemical Biology and Drug Design*, **2019**, 93, 1083-1095	2.9	10
202	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
201	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
200	Diagrams for comprehensive molecular orbital-based chemical reaction analyses: reactive orbital energy diagrams. *Physical Chemistry Chemical Physics*, **2018**, 20, 14211-14222	3.6	3
199	Planar pentacoordinate carbon in CGa derivatives. *Physical Chemistry Chemical Physics*, **2018**, 20, 12350-12355	3.6	27
198	Tunneling and quantum localization in chaos-driven symmetric triple well potential: An approach using quantum theory of motion. *International Journal of Quantum Chemistry*, **2018**, 118, e25531	2.1	1
197	A (TP) phase diagram for the adsorption/desorption of carbon dioxide and hydrogen in a Cu(II)-MOF. *Polyhedron*, **2018**, 153, 254-260	2.7	4
196	Exohedral complexation of B39- with ECp*+ half-sandwich complexes (E Si, Ge, Sn, Pb): A DFT study. *Computational and Theoretical Chemistry*, **2018**, 1140, 49-55	2	1
195	Noble Gas Inserted Metal Acetylides (Metal = Cu, Ag, Au). *Journal of Physical Chemistry A*, **2018**, 122, 7391-7401	2.8	20
194	Confinement induced catalytic activity in a Diels-Alder reaction: comparison among various CB[n], n = 6-8, cavitands. *Journal of Molecular Modeling*, **2018**, 24, 228	2	5
193	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
192	Reactions involving some gas molecules through sequestration on Al Be cluster: An electron density based study. *Journal of Computational Chemistry*, **2018**, 39, 535-545	3.5	3
191	Host-guest interactions between octa acid and cations/nucleobases. *Journal of Computational Chemistry*, **2018**, 39, 161-175	3.5	10
190	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
189	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

188	Noble gas encapsulated B cage. *Physical Chemistry Chemical Physics*, **2018**, 20, 1953-1963	3.6	29
187	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	2.5	1
186	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
185	HNgBeF3 (Ng = Ar-Rn): Superhalogen-supported noble gas insertion compounds. *International Journal of Quantum Chemistry*, **2018**, 118, e25499	2.1	11
184	Hydrogen Storage in All-Metal and Nonmetal Aromatic Clusters **2018**, 329-362		
183	Adsorption of Molecular Hydrogen on Lithium Phosphorus Double-Helices. *Journal of Physical Chemistry C*, **2018**, 122, 27941-27946	3.8	7
182	Activation of Small Molecules (H, CO, NO, CH, and CH) by a Porphyrinoid-Based Dimagnesium(I) Complex, an Electride. *ACS Omega*, **2018**, 3, 17199-17211	3.9	9
181	Stabilization of Boron-Boron Triple Bonds by Mesoionic Carbenes. *ACS Omega*, **2018**, 3, 13720-13730	3.9	13
180	Analyzing torquoselectivity in a series of unusual ring-opening reactions through bond reactivity indices and the adaptive natural density partitioning method. *International Journal of Quantum Chemistry*, **2018**, 118, e25778	2.1	4
179	Ligand-Supported E Clusters (E=Si-Sn). *Chemistry - A European Journal*, **2017**, 23, 7463-7473	4.8	10
178	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
177	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
176	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
175	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
174	Modeling of 1-D Nanowires and analyzing their Hydrogen and Noble Gas Binding Ability. *Journal of Chemical Sciences*, **2017**, 129, 849-858	1.8	7
173	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
172	The strongest CO binding and the highest C-O stretching frequency. *Physical Chemistry Chemical Physics*, **2017**, 19, 2286-2293	3.6	14
171	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	2

170	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
169	Change in optoelectronic properties of ExBox on functionalization and guest encapsulation. *Physical Chemistry Chemical Physics*, **2017**, 19, 23373-23385	3.6	9
168	Endohedral gas adsorption by cucurbit[7]uril: a theoretical study. *Physical Chemistry Chemical Physics*, **2017**, 19, 24448-24452	3.6	13
167	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	3.2	
166	Finite temperature grand canonical ensemble study of the minimum electrophilicity principle. *Journal of Chemical Physics*, **2017**, 147, 124103	3.9	23
165	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
164	Role of Lithium Decoration on Hydrogen Storage Potential **2017**, 56,		2
163	Quantitative Structure-Activity/Property/Toxicity Relationships through Conceptual Density Functional Theory-Based Reactivity Descriptors **2017**, 1517-1572		3
162	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
161	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
160	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	3.8	6
159	Noble Gas Binding Ability of Metal-Bipyridine Monocationic Complexes (Metal=Cu, Ag, Au): A Computational Study. *ChemistrySelect*, **2016**, 1, 5842-5849	1.8	16
158	Encapsulation of small gas molecules and rare gas atoms inside the octa acid cavitand. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	24
157	Optical response and gas sequestration properties of metal cluster supported graphene nanoflakes. *Physical Chemistry Chemical Physics*, **2016**, 18, 18811-27	3.6	21
156	Selectivity in Gas Adsorption by Molecular Cucurbit[6]uril. *Journal of Physical Chemistry C*, **2016**, 120, 13911-13921	3.8	35
155	How strong are the metallocene-metallocene interactions? Cases of ferrocene, ruthenocene, and osmocene. *Physical Chemistry Chemical Physics*, **2016**, 18, 550-6	3.6	28
154	Structure and bonding of IrB12□converting a rigid boron B12 platelet to a Wankel motor. *RSC Advances*, **2016**, 6, 27177-27182	3.7	56
153	Viability of aromatic all-pnictogen anions. *Physical Chemistry Chemical Physics*, **2016**, 18, 11738-45	3.6	3

152	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
151	Statistical Significance of the Maximum Hardness Principle Applied to Some Selected Chemical Reactions. *Molecules*, **2016**, 21,	4.8	6
150	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
149	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
148	Solution of the Classical Schrödinger equation for a driven symmetric triple well: A comparison with its classical counterpart. *International Journal of Quantum Chemistry*, **2016**, 116, 1224-1243	2.1	6
147	Possible sequestration of polar gas molecules by superhalogen supported aluminum nitride nanoflakes. *Journal of Molecular Modeling*, **2016**, 22, 271	2	3
146	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
145	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
144	Noble gas supported B3+ cluster: formation of strong covalent noble gas–boron bonds. *RSC Advances*, **2016**, 6, 78611-78620	3.7	26
143	Scaling properties of information-theoretic quantities in density functional reactivity theory. *Physical Chemistry Chemical Physics*, **2015**, 17, 4977-88	3.6	59
142	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
141	Interaction of BN- and BP-doped graphene nanoflakes with some representative neutral molecules and anions. *Molecular Physics*, **2015**, 113, 2916-2929	1.7	
140	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
139	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
138	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
137	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
136	Hydrogen trapping potential of (HF)m (m=1–8) and (H2O)n (n=1–10) clusters. *Computational and Theoretical Chemistry*, **2015**, 1071, 18-26	2	3
135	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

134	Metastable behavior of noble gas inserted tin and lead fluorides. *Physical Chemistry Chemical Physics*, **2015**, 17, 972-82	3.6	45
133	Dynamical behavior of Borospherene: A Nanobubble. *Scientific Reports*, **2015**, 5, 11287	4.9	70
132	Fermi accelerator: A new insight from quantum theory of motion. *International Journal of Quantum Chemistry*, **2015**, 115, 1733-1738	2.1	3
131	Three-dimensional networks containing rectangular Sr4 and Ba4 units: Synthesis, structure, bonding, and potential application for Ne gas separation. *International Journal of Quantum Chemistry*, **2015**, 115, 1501-1510	2.1	6
130	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
129	Orbital free DFT versus single density equation: a perspective through quantum domain behavior of a classically chaotic system. *Physical Chemistry Chemical Physics*, **2015**, 17, 31516-29	3.6	7
128	Quantitative Structure-Activity/Property/Toxicity Relationships through Conceptual Density Functional Theory-Based Reactivity Descriptors. *Advances in Chemical and Materials Engineering Book Series*, **2015**, 123-179	0.2	
127	Cucurbit[6]uril: A Possible Host for Noble Gas Atoms. *Journal of Physical Chemistry B*, **2015**, 119, 10962-74	3.4	41
126	Confinement induced binding in noble gas atoms within a BN-doped carbon nanotube. *Chemical Physics Letters*, **2015**, 621, 29-34	2.5	26
125	Unique bonding pattern and resulting bond stretch isomerism in. *International Journal of Quantum Chemistry*, **2015**, 115, 426-433	2.1	8
124	Reactivity dynamics of confined atoms in the presence of an external magnetic field. *European Physical Journal D*, **2014**, 68, 1	1.3	17
123	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
122	Confinement of (HF)2 in Cn (n = 60, 70, 80, 90) cages. *Chemical Physics Letters*, **2014**, 616-617, 49-54	2.5	10
121	Gas storage potential of ExBox⊞ and its Li-decorated derivative. *Physical Chemistry Chemical Physics*, **2014**, 16, 21964-79	3.6	10
120	Noble gas encapsulation: clathrate hydrates and their HF doped analogues. *Physical Chemistry Chemical Physics*, **2014**, 16, 17943-54	3.6	18
119	Metal (copper) segregation in magmas. *Lithos*, **2014**, 208-209, 462-470	2.9	8
118	B18(2-): a quasi-planar bowl member of the Wankel motor family. *Chemical Communications*, **2014**, 50, 8140-3	5.8	98
117	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

116	Stability of noble-gas-bound SiH_4 clusters. *ChemPhysChem*, **2014**, 15, 3554-64	3.2	29
115	The inorganic analogues of carbo -benzene. *Chemical Physics Letters*, **2014**, 610-611, 209-212	2.5	8
114	Confinement induced binding of noble gas atoms. *Journal of Chemical Physics*, **2014**, 140, 164306	3.9	48
113	Chemical reactivity through structure-stability landscape. *International Journal of Quantum Chemistry*, **2014**, 114, 1421-1429	2.1	5
112	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
111	Stability and structural dynamics of Be32- clusters. *Chemical Physics Letters*, **2014**, 593, 128-131	2.5	10
110	Carbo-cages: a computational study. *Journal of Organic Chemistry*, **2014**, 79, 5463-70	4.2	12
109	Quantum equivalence of a driven triple-well Van der Pol oscillator: A QTM study. *Chemical Physics*, **2014**, 438, 7-15	2.3	6
108	Host-guest interactions in ExBox4+. *ChemPhysChem*, **2014**, 15, 4108-16	3.2	15
107	Bohmian trajectory from the "classical" Schrödinger equation. *Chaos*, **2014**, 24, 043123	3.3	6
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