Mahdi D Esrafili

List of Publications by Year
in descending order

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339	6,435	81900	182427
papers	citations	39 h-index	51 g-index

344	344	344	3601
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	New page to access pyridine derivatives: synthesis from N-propargylamines. RSC Advances, 2016, 6, 71662-71675.	3.6	81
2	Exploring different reaction mechanisms for oxidation of CO over a single Pd atom incorporated nitrogen-doped graphene: A DFT study. Applied Surface Science, 2019, 463, 526-534.	6.1	76
3	Novel routes to quinoline derivatives from N-propargylamines. RSC Advances, 2016, 6, 49730-49746.	3.6	73
4	A Comparative Study of CO Oxidation on Nitrogenâ€•and PhosphorusâÐoped Graphene. ChemPhysChem, 2015, 16, 3719-3727.	2.1	70
5	A comparative DFT study on the CO oxidation reaction over Al- and Ge-embedded graphene as efficient metal-free catalysts. Applied Surface Science, 2016, 378, 418-425.	6.1	69
6	A DFT study on electronic and optical properties of aspirin-functionalized B12N12 fullerene-like nanocluster. Structural Chemistry, 2017, 28, 735-748.	2.0	68
7	A density functional theory study on the adsorption and decomposition of methanol on B12N12 fullerene-like nanocage. Superlattices and Microstructures, 2014, 67, 54-60.	3.1	67
8	Characteristics and nature of halogen bonds in linear clusters of NCX (X=Cl, and Br): anab initio, NBO and QTAIM study. Molecular Physics, 2011, 109, 2451-2460.	1.7	66
9	Insights into the strength and nature of carbeneÂ·Â·Â·halogen bond interactions: a theoretical perspective. Journal of Molecular Modeling, 2013, 19, 2559-2566.	1.8	63
10	Theoretical insights into hydrogenation of CO2 to formic acid over a single Co atom incorporated nitrogen-doped graphene: A DFT study. Applied Surface Science, 2019, 475, 363-371.	6.1	63
11	Functional group effect of isoreticular metalâ€“organic frameworks on heavy metal ion adsorption. New Journal of Chemistry, 2018, 42, 8864-8873.	2.8	62
12	Methylamine adsorption and decomposition on B12N12 nanocage: A density functional theory study. Surface Science, 2014, 626, 44-48.	1.9	61
13	Nitrogen-doped (6,0) carbon nanotubes: A comparative DFT study based on surface reactivity descriptors. Computational and Theoretical Chemistry, 2013, 1015, 1-7.	2.5	59
14	Hybrid sol-gel coatings based on silanes-amino acids for corrosion protection of AZ91 magnesium alloy: Electrochemical and DFT insights. Progress in Organic Coatings, 2019, 131, 191-202.	3.9	59
15	Si-doped graphene: A promising metal-free catalyst for oxidation of SO2. Chemical Physics Letters, 2016, 649, 37-43.	2.6	57
16	A theoretical investigation on the nature of Clâ‹¯N and Brâ‹¯N halogen bonds in FArXâ‹¯NCY complexes (X=Cl,) Tj ETQq0 0 0 rgBT /Overlo	2.5	56
17	Investigation of H-bonding and halogen-bonding effects in dichloroacetic acid: DFT calculations of NQR parameters and QTAIM analysis. Journal of Molecular Modeling, 2012, 18, 5005-5016.	1.8	55
18	Potential of C-doped boron nitride fullerene as a catalyst for methanol dehydrogenation. Computational Materials Science, 2014, 92, 172-177.	3.0	55

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19	An ab initio study on chalcogenâ€“chalcogen bond interactions in cyclic (SHX)3 complexes (X=F, Cl, CN,) Tj ETQq1 1 0.784314 rgBT	2.6	54
20	Tetrel bond cooperativity in open-chain (CH3CN)n and (CH3NC)n clusters (n=2â€“7): An ab initio study. Chemical Physics Letters, 2015, 628, 16-20.	2.6	54
21	Mutual interplay between pnicogen bond and dihydrogen bond in HMHâ‹¯HCNâ‹¯PH2X complexes (M=Be, Mg,) Tj ETQq1 1 0.784314	2.5	52
22	Sn-embedded graphene: An active catalyst for CO oxidation to CO 2 ?. Physica E: Low-Dimensional Systems and Nanostructures, 2015, 74, 382-387.	2.7	52
23	Bifurcated chalcogen bonds: A theoretical study on the structure, strength and bonding properties. Chemical Physics Letters, 2015, 634, 210-215.	2.6	52
24	A theoretical evidence for mutual influence between SÂ·Â·Â·N(C) and hydrogen/lithium/halogen bonds: competition and interplay between Ï€-hole and Ïƒ-hole interactions. Structural Chemistry, 2014, 25, 1197-1205.	2.0	51
25	Theoretical study of Nâ€“HÂ· Â· Â·O hydrogen bonding properties and cooperativity effects in linear acetamide clusters. Theoretical Chemistry Accounts, 2008, 121, 135-146.	1.4	50
26	Pd-embedded graphene: An efficient and highly active catalyst for oxidation of CO. Superlattices and Microstructures, 2016, 92, 60-67.	3.1	50
27	The selective adsorption of formaldehyde and methanol over Al- or Si-decorated graphene oxide: A DFT study. Journal of Molecular Graphics and Modelling, 2018, 80, 25-31.	2.4	49
28	New route to 1,4-oxazepane and 1,4-diazepane derivatives: synthesis from N-propargylamines. RSC Advances, 2016, 6, 99781-99793.	3.6	48
29	A DFT study on the N₂O reduction by CO molecule over silicon carbide nanotubes and nanosheets. RSC Advances, 2016, 6, 59091-59099.	3.6	46
30	Revealing substitution effects on the strength and nature of halogen-hydride interactions: a theoretical study. Journal of Molecular Modeling, 2013, 19, 3767-3777.	1.8	45
31	A theoretical study of substitution effects on halogenâ€“Ï€ interactions. Molecular Physics, 2014, 112, 1160-1166.	1.7	44
32	Cooperative effects in pnicogen bonding: (PH2F)2â€“7 and (PH2Cl)2â€“7 clusters. Chemical Physics Letters, 2014, 609, 37-41.	2.6	44
33	Strong Tetrel Bonds: Theoretical Aspects and Experimental Evidence. Molecules, 2018, 23, 2642.	3.8	43
34	Boron and nitrogen co-doped graphene nanosheets for NO and NO2 gas sensing. Physics Letters, Section A: General, Atomic and Solid State Physics, 2019, 383, 1607-1614.	2.1	43
35	Characteristics and nature of the intermolecular interactions in boron-bonded complexes with carbene as electron donor: an ab initio, SAPT and QTAIM study. Journal of Molecular Modeling, 2012, 18, 2003-2011.	1.8	42
36	Carbon-doped boron nitride nanosheets as highly sensitive materials for detection of toxic NO and NO2 gases: A DFT study. Vacuum, 2019, 166, 127-134.	3.5	42

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37	A DFT study on carbon-doping at different sites of (8, 0) boron nitride nanotube. Structural Chemistry, 2013, 24, 573-581.	2.0	41
38	Cooperativity effects betweenÏƒ-hole interactions: a theoretical evidence for mutual influence between chalcogen bond and halogen bond interactions in F₂SÂ·Â·Â·NCXÂ·Â·Â·NCY complexes (X =) Tj ETQq0 0 0 rgBT /Ov	1.7	41
39	Does single-electron chalcogen bond exist? Some theoretical insights. Journal of Molecular Modeling, 2015, 21, 65.	1.8	41
40	Electric field assisted activation of CO2 over P-doped graphene: A DFT study. Journal of Molecular Graphics and Modelling, 2019, 90, 192-198.	2.4	41
41	Enhanced adsorptive removal of Indigo carmine dye performance by functionalized carbon nanotubes based adsorbents from aqueous solution: equilibrium, kinetic, and DFT study. Journal of Nanostructure in Chemistry, 2019, 9, 323-334.	9.1	41
42	A comparative study on carbon, boron-nitride, boron-phosphide and silicon-carbide nanotubes based on surface electrostatic potentials and average local ionization energies. Journal of Molecular Modeling, 2013, 19, 2375-2382.	1.8	40
43	Theoretical insight into cooperativity in lithium-bonded complexes: Linear clusters of LiCN and LiNC. Chemical Physics Letters, 2013, 577, 6-10.	2.6	40
44	Catalytic hydrogenation of CO 2 over Pt- and Ni-doped graphene: A comparative DFT study. Journal of Molecular Graphics and Modelling, 2017, 77, 143-152.	2.4	40
45	Boosting graphene reactivity with co-doping of boron and nitrogen atoms: CO oxidation by O2 molecule. Applied Surface Science, 2018, 455, 808-814.	6.1	40
46	Computational study on the characteristics of the interaction in linear urea clusters. International Journal of Quantum Chemistry, 2011, 111, 3184-3195.	2.0	39
47	A theoretical investigation of the characteristics of hydrogen/halogen bonding interactions in dibromo-nitroaniline. Journal of Molecular Modeling, 2013, 19, 1417-1427.	1.8	39
48	Investigation of substituent effects in aerogenâ€bonding interaction between ZO₃ (Z=Kr,) Tj ETQq0 0 0 rgBT /Overlock 10	2.0	39
49	Carbon-doped boron nitride nanosheet as a promising catalyst for N2O reduction by CO or SO2 molecule: A comparative DFT study. Applied Surface Science, 2018, 444, 584-589.	6.1	39
50	Experimental and theoretical study of TiO2 based nanostructured semiconducting humidity sensor. Ceramics International, 2019, 45, 8362-8369.	4.8	39
51	Molecular dynamics simulations of choline chloride and phenyl propionic acid deep eutectic solvents: Investigation of structural and dynamics properties. Journal of Molecular Graphics and Modelling, 2021, 106, 107908.	2.4	39
52	Density Functional Theory Investigation of Hydrogen Bonding Effects on the Oxygen, Nitrogen and Hydrogen Electric Field Gradient and Chemical Shielding Tensors of Anhydrous Chitosan Crystalline Structure. Journal of Physical Chemistry A, 2007, 111, 963-970.	2.5	38
53	Theoretical study of the interplay between halogen bond and lithiumâ€“Ï€ interactions: Cooperative and diminutive effects. Chemical Physics Letters, 2013, 588, 47-50.	2.6	38
54	A DFT study on the catalytic hydrogenation of CO2 to formic acid over Ti-doped graphene nanoflake. Chemical Physics Letters, 2017, 682, 49-54.	2.6	38

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55	A structural study of fentanyl by DFT calculations, NMR and IR spectroscopy. Journal of Molecular Structure, 2017, 1128, 552-562.	3.6	38
56	Density functional theory study of atomic oxygen, O2 and O3 adsorptions on the H-capped (5,0) single-walled carbon nanotube. Physica E: Low-Dimensional Systems and Nanostructures, 2009, 41, 1373-1378.	2.7	37
57	DFT study of NH3 adsorption on the (5,0), (8,0), (5,5) and (6,6) single-walled carbon nanotubes. Calculated binding energies, NMR and NQR parameters. Physica B: Condensed Matter, 2010, 405, 1455-1460.	2.7	37
58	A DFT study on the possibility of using boron nitride nanotubes as a dehydrogenation catalyst for methanol. Applied Surface Science, 2014, 314, 90-96.	6.1	37
59	Intriguing properties of unusual silicon nanocrystals. RSC Advances, 2015, 5, 78192-78208.	3.6	37
60	A theoretical evidence for cooperative enhancement in aerogen-bonding interactions: Open-chain clusters of KrOF2 and XeOF2. Chemical Physics Letters, 2016, 662, 80-85.	2.6	36
61	NO reduction by CO molecule over Si-doped boron nitride nanosheet: A dispersion-corrected DFT study. Chemical Physics Letters, 2018, 695, 131-137.	2.6	36
62	Influence of Nâ€“Hâ€¦O and Oâ€“Hâ€¦O hydrogen bonds on the 17O, 15N and 13C chemical shielding tensors in crystalline acetaminophen: A density functional theory study. Biophysical Chemistry, 2007, 128, 38-45.	2.8	35
63	Structure, bonding, electronic and energy aspects of a new family of early lanthanide (La, Ce and Nd) complexes with phosphoric triamides: Insights from experimental and DFT studies. Dalton Transactions, 2012, 41, 1597-1608.	3.3	35
64	Can Si-embedded boron nitride nanotubes act as a favorable metal-free catalyst for CO oxidation by N₂O?. RSC Advances, 2015, 5, 100290-100298.	3.6	35
65	Ab initio calculations of cooperativity effects on chalcogen bonding: linear clusters of (OCS)2â€“8 and (OCSe)2â€“8. Structural Chemistry, 2015, 26, 199-206.	2.0	35
66	N 2 O reduction over a fullerene-like boron nitride nanocage: A DFT study. Physics Letters, Section A: General, Atomic and Solid State Physics, 2017, 381, 2085-2091.	2.1	35
67	Graphene-Based Electrochemical Supercapacitors. Interface Science and Technology, 2019, 27, 339-386.	3.3	35
68	Preparation and characterization of a new waste-derived mesoporous carbon structure for ultrahigh adsorption of benzene and toluene at ambient conditions. Journal of Hazardous Materials, 2020, 384, 121317.	12.4	35
69	Cooperativity of tetrel bonds tuned by substituent effects. Molecular Physics, 2016, 114, 1528-1538.	1.7	34
70	Chalcogen bonds formed through Ï€-holes: SO₃ complexes with nitrogen and phosphorus bases. Molecular Physics, 2016, 114, 276-282.	1.7	34
71	A computational study of water adsorption on boron nitride nanotube. Structural Chemistry, 2010, 21, 903-908.	2.0	33
72	A DFT study of pyrazine derivatives and their Fe complexes in corrosion inhibition process. Journal of Molecular Structure, 2015, 1086, 64-72.	3.6	33

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73	A DFT study on the central-ring doped HBC nanographenes. Journal of Molecular Graphics and Modelling, 2017, 73, 101-107.	2.4	33
74	Development of TiO2 nanofibers based semiconducting humidity sensor: adsorption kinetics and DFT computations. Materials Chemistry and Physics, 2020, 239, 121981.	4.0	33
75	14N and 17O electric field gradient tensors in benzamide clusters: Theoretical evidence for cooperative and electronic delocalization effects in Nâ€“Hâ‹¯O hydrogen bonding. Chemical Physics, 2008, 348, 175-180.	1.9	32
76	Al- or Si-decorated graphene oxide: A favorable metal-free catalyst for the N2O reduction. Applied Surface Science, 2016, 387, 454-460.	6.1	32
77	Theoretical 14N nuclear quadrupole resonance parameters for sulfa drugs: Sulfamerazine and sulfathiazole. Journal of Molecular Graphics and Modelling, 2008, 27, 326-331.	2.4	31
78	Anionic tetrel bonds: An ab initio study. Chemical Physics Letters, 2018, 691, 394-400.	2.6	31
79	A theoretical study of 17O, 14N and 2H nuclear quadrupole coupling tensors in the real crystalline structure of acetaminophen. Chemical Physics, 2007, 333, 97-104.	1.9	30
80	Oxidation of CO by N₂O over Al- and Ti-doped graphene: a comparative study. RSC Advances, 2016, 6, 64832-64840.	3.6	29
81	Density functional theory study of Nâ€“Hâ‹¯O, Oâ€“Hâ‹¯O and Câ€“Hâ‹¯O hydrogen-bonding effects on the 14N and 2H nuclear quadrupole coupling tensors of N-acetyl-valine. Biophysical Chemistry, 2008, 133, 11-18.	2.8	28
82	A DFT study on SO3 capture and activation over Si- or Al-doped graphene. Chemical Physics Letters, 2016, 658, 146-151.	2.6	28
83	Theoretical insights into nature of Ï€-hole interactions between triel centers (B and Al) and radical methyl as a potential electron donor: Do single-electron triel bonds exist?. Structural Chemistry, 2016, 27, 1157-1164.	2.0	28
84	Are choline chloride-based deep eutectic solvents better than methyl diethanolamine solvents for natural gas Sweetening? theoretical insights from molecular dynamics simulations. Journal of Molecular Liquids, 2021, 338, 116716.	4.9	28
85	DFT calculations on the catalytic oxidation of CO over Si-doped (6,0) boron nitride nanotubes. Structural Chemistry, 2016, 27, 595-604.	2.0	27
86	Defect engineering-induced porosity in graphene quantum dots embedded metal-organic frameworks for enhanced benzene and toluene adsorption. Journal of Hazardous Materials, 2021, 416, 125973.	12.4	27
87	Si-embedded boron-nitride nanotubes as an efficient and metal-free catalyst for NO oxidation. Superlattices and Microstructures, 2015, 81, 7-15.	3.1	26
88	N2O + SO2 reaction over Si- and C-doped boron nitride nanotubes: A comparative DFT study. Applied Surface Science, 2017, 403, 43-50.	6.1	26
89	The triel bond: a potential force for tuning anionâ€“Ï€ interactions. Molecular Physics, 2018, 116, 388-398.	1.7	26
90	BN co-doped graphene monolayers as promising metal-free catalysts for N 2 O reduction: A DFT study. Chemical Physics Letters, 2018, 705, 44-49.	2.6	26

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91	A Single Pd Atom Stabilized on Boronâ€Vacancy of hâ€BN Nanosheet: A Promising Catalyst for CO Oxidation. ChemistrySelect, 2018, 3, 9181-9188.	1.5	26
92	Computational mechanistic insights into CO oxidation reaction over Fe decorated C24N24 fullerene. Inorganic Chemistry Communication, 2019, 106, 190-196.	3.9	26
93	A DFT study on doping assisted changing of B80 electronic structure: Promising candidates for NH3 sensor. Sensors and Actuators B: Chemical, 2014, 191, 457-463.	7.8	25
94	Probing reaction pathways for oxidation of CO by O2 molecule over P-doped divacancy graphene: A DFT study. Applied Surface Science, 2018, 440, 580-585.	6.1	25
95	Tuning of pnicogen and chalcogen bonds by an aerogen-bonding interaction: a comparative ab initio study. Molecular Physics, 2019, 117, 58-66.	1.7	25
96	Enhancement effect of lithium bonding on the strength of pnicogen bonds: XH₂PÂ·Â·Â·NCLiÂ·Â·Â·NCY as a working model (X = F, Cl; Y = H, F, Cl, CN). Molecular Physics, 2014, 112, 2058-2062.	1.7	24
97	Single-electron aerogen bonds: Do they exist?. Chemical Physics Letters, 2016, 659, 196-202.	2.6	24
98	Adsorption and decomposition of formaldehyde on the B12N12 nanostructure: a density functional theory study. Monatshefte FÃ¼r Chemie, 2017, 148, 1727-1731.	1.8	24
99	Adsorptive mercaptan removal of liquid phase using nanoporous graphene: Equilibrium, kinetic study and DFT calculations. Ecotoxicology and Environmental Safety, 2018, 165, 533-539.	6.0	24
100	NO electrochemical reduction over Si-N4 embedded graphene: A DFT investigation. Applied Surface Science, 2021, 544, 148869.	6.1	24
101	Exploring the structural and transport properties of glyceline DES-Based boron nitride nanotube Nanofluid: The effects of nanotube diameter. Journal of Molecular Liquids, 2021, 341, 117277.	4.9	24
102	Synthesis, structural characterization and DFT calculations of a new one-dimensional diorganotin(IV) derivative of N-isonicotinyl phosphoramide. Polyhedron, 2014, 71, 8-16.	2.2	23
103	Application of Si-doped graphene as a metal-free catalyst for decomposition of formic acid: A theoretical study. International Journal of Quantum Chemistry, 2015, 115, 1153-1160.	2.0	23
104	Exploring â€œaerogenâ€“hydrideâ€•interactions between ZOF2 (Z = Kr, Xe) and metal hydrides: An ab initio study. Chemical Physics Letters, 2016, 654, 23-28.	2.6	23
105	A comparative study of the CO oxidation reaction over pristine and C-doped boron nitride fullerene. RSC Advances, 2016, 6, 17172-17178.	3.6	23
106	Catalytic reduction of NO by CO molecules over Ni-doped graphene: a DFT investigation. New Journal of Chemistry, 2017, 41, 13149-13155.	2.8	23
107	Optical and photocatalytic characteristics of Al and Cu doped TiO2: Experimental assessments and DFT calculations. Journal of Physics and Chemistry of Solids, 2022, 161, 110404.	4.0	23
108	Mutual influence between anionâ€“Ï€ and pnicogen bond interactions: The enhancement of Pâ‹¯N and Pâ‹¯O interactions by an anionâ€“Ï€ bond. Journal of Molecular Graphics and Modelling, 2015, 57, 99-105.	2.4	22

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109	Pnicogenâ€“pnicogen interactions in O2XP:PH2Y complexes (X=H, F, CN; Y=H, OH, OCH3, CH3, NH2). Chemical Physics Letters, 2015, 638, 122-127.	2.6	22
110	Strengthening of the halogen-bonding by an aerogen bond interaction: substitution and cooperative effects in O₃ZÂ·Â·Â·NCXÂ·Â·Â·NCY (Z = Ar, Kr, Xe; X = Cl, Br, I; Y = H, F, OH) complexes. Molecular Physics, 2016, 114, 2177-2186.	1.7	22
111	Unusual cooperativity effects between halogen bond and donor-acceptor interactions: The role of orbital interaction. Chemical Physics Letters, 2017, 678, 275-282.	2.6	22
112	A DFT study on NO reduction to N2O using Al- and P-doped hexagonal boron nitride nanosheets. Journal of Molecular Graphics and Modelling, 2019, 89, 41-49.	2.4	22
113	How do phosphoramides compete with phosphine oxides in lanthanide complexation? Structural, electronic and energy aspects at ab initio and DFT levels. Theoretical Chemistry Accounts, 2010, 127, 539-550.	1.4	21
114	Cooperative interaction between Ï€-hole and single-electronÏƒ-hole interactions in O2SÂ·Â·Â·NCXÂ·Â·Â·CH3and O2SeÂ·Â·Â·NCXÂ·Â·Â·CH3complexes (X = F, Cl, Br and I). Molecular Physics, 2014, 112, 2078-2084.	1.7	20
115	The dual role of halogen, chalcogen, and pnictogen atoms as Lewis acid and base: Triangular XBr:SHX:PH₂ X complexes (Xâ€‰=â€‰F, Cl, Br, CN, NC, OH, NH₂ , and OCH₃) Tj ETQq1 1 0.78	2.0	20
116	An ab initio study on tunability of Ïƒ-hole interactions in XHS:PH2Y and XH2P:SHY complexes (Xâ€‰=â€‰F, Cl, Br) Tj ETQq0 0 0 rgBT /	1.8	20
117	Catalytic dehydrogenation of hydrazine on silicon-carbide nanotubes: A DFT study on the kinetic issue. Surface Science, 2015, 632, 118-125.	1.9	20
118	B-doped C3N monolayer: a robust catalyst for oxidation of carbon monoxide. Theoretical Chemistry Accounts, 2019, 138, 1.	1.4	20
119	B-, N-doped and BN codoped C₆₀ heterofullerenes for environmental monitoring of NO and NO₂: a DFT study. Molecular Physics, 2020, 118, .	1.7	20
120	Effects of B and N doping/codoping on the adsorption behavior of C60 fullerene towards aspirin: A DFT investigation. Journal of Molecular Liquids, 2021, 342, 117459.	4.9	20
121	Efficient dehydrogenation of formic acid using Al 12 N 12 nanocage: A DFT study. Superlattices and Microstructures, 2014, 75, 17-26.	3.1	19
122	Cooperative effects between tetrel bond and other Ïƒâ€“hole bond interactions: a comparative investigation. Molecular Physics, 2015, 113, 3703-3711.	1.7	19
123	Interplay between hydrogen bond and single-electron tetrel bond: H3Câ‹¯COX2â‹¯HY and H3Câ‹¯CSX2â‹¯HY (X = F,) Tj ETQq1 1 0.784 101-106.	2.5	19
124	A first-principles study on the adsorption behaviour of methanol and ethanol over C₅₉B heterofullerene. Molecular Physics, 2017, 115, 1633-1641.	1.7	19
125	A DFT study on the potential application of Si@C24N24 porous fullerene as an innovative and highly active catalyst for NO reduction. Chemical Physics Letters, 2019, 724, 80-85.	2.6	19
126	Theoretical study on cooperative effects between Xâ‹¯N and Xâ‹¯Carbene halogen bonds (Xâ€‰=â€‰F,Cl,Br and I). Journal of Molecular Modeling, 2013, 19, 4797-4804.	1.8	18

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127	Competition and interplay between the lithium bonding and hydrogen bonding: R3CÂ·Â·Â·HYÂ·Â·Â·LiY and R3CÂ·Â·Â·LiYÂ·Â·Â·HY triads as a working model (R=H, CH3; Y=CN, NC). Journal of Molecular Modeling, 2013, 19, 5031-5035.	1.8	18
128	An ab initio study on the concerted interaction between chalcogen and pnicogen bonds. Journal of Molecular Modeling, 2014, 20, 2545.	1.8	18
129	Cooperative and diminutive interplay between the sodium bonding with hydrogen and dihydrogen bondings in ternary complexes of NaC₃N with HMgH and HCN (HNC). Molecular Physics, 2014, 112, 2017-2022.	1.7	18
130	A theoretical evidence for cooperativity effects in fluorine-centered halogen bonds: linear (FCN)2â€“7 and (FNC)2â€“7 clusters. Structural Chemistry, 2014, 25, 403-408.	2.0	18
131	Exploring Ïƒ-hole bonding in XH3SiÎ‡Î‡HMY (X=H, F, CN; M=Be, Mg; Y=H, F, CH3) complexes: a â€œtetrel-hydrideâ€• interaction. Journal of Molecular Modeling, 2015, 21, 60.	1.8	18
132	An ab initio study on the nature of Ïƒ-hole interactions in pnicogen-bonded complexes with carbene as an electron donor. Molecular Physics, 2016, 114, 2115-2122.	1.7	18
133	Ïƒ-Hole bond tunability in YO2X2:NH3 and YO2X2:H2O complexes (XÂ=ÂF, Cl, Br; YÂ=ÂS, Se): trends and theoretical aspects. Structural Chemistry, 2016, 27, 617-625.	2.0	18
134	An ab initio study on anionic aerogen bonds. Chemical Physics Letters, 2017, 667, 337-344.	2.6	17
135	A computational study on the strength and nature of bifurcated aerogen bonds. Chemical Physics Letters, 2018, 698, 1-6.	2.6	17
136	CO Oxidation Catalyzed by a Single Ti Atom Supported on Divacancy Defective Graphene: A Dispersionâ€Corrected DFT Study. ChemistrySelect, 2018, 3, 4471-4479.	1.5	17
137	A DFT study on the possibility of using a single Cu atom incorporated nitrogenâ€doped graphene as a promising and highly active catalyst for oxidation of CO. International Journal of Quantum Chemistry, 2019, 119, e25857.	2.0	17
138	Substituent effects on cooperativity of pnicogen bonds. Journal of Molecular Modeling, 2014, 20, 2436.	1.8	16
139	Substituent effects on cooperativity between lithium bonds. International Journal of Quantum Chemistry, 2014, 114, 295-301.	2.0	16
140	Triphenyltin(<scp>iv</scp>) adducts of diphosphoryl ligands: structural, electronic and energy aspects from X-ray crystallography and theoretical calculations. RSC Advances, 2015, 5, 17482-17492.	3.6	16
141	The strengthening effect of a hydrogen or lithium bond on the ZÂ·Â·Â·N aerogen bond (Z = Ar, Kr and Xe): a comparative study. Molecular Physics, 2016, 114, 3265-3276.	1.7	16
142	Anab initiostudy on competition between pnicogen and chalcogen bond interactions in binary XHS:PH₂X complexes (X = F, Cl, CCH, COH, CH₃, OH, OCH₃and) Tj ETQq0 0 0 rgBT /Overlock 10	1.7	16
143	Potential of Si-doped boron nitride nanotubes as a highly active and metal-free electrocatalyst for oxygen reduction reaction: A DFT study. Synthetic Metals, 2017, 226, 129-138.	3.9	16
144	Epoxidation of ethylene over Pt-, Pd- and Ni-doped graphene in the presence of N₂O as an oxidant: a comparative DFT study. New Journal of Chemistry, 2017, 41, 9815-9825.	2.8	16

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145	Adsorption of formamide over pristine and Al-doped boron nitride nanosheets: A dispersion-corrected DFT study. Journal of Molecular Graphics and Modelling, 2018, 82, 101-107.	2.4	16
146	A comparative DFT study on single-atom catalysis of CO oxidation over Al- and P-embedded hexagonal boron-nitride nanosheets. Journal of Molecular Graphics and Modelling, 2018, 85, 323-330.	2.4	16
147	Efficient DBT removal from diesel oil by CVD synthesized N-doped graphene as a nanoadsorbent: Equilibrium, kinetic and DFT study. Ecotoxicology and Environmental Safety, 2019, 172, 89-96.	6.0	16
148	Oxidation of SO2 over C-doped boron nitride nanosheets: The role of C-doping, and solvent effects. Journal of Molecular Graphics and Modelling, 2019, 86, 209-218.	2.4	16
149	Alcohol Oxidation and Hydrogen Evolution. Interface Science and Technology, 2019, 27, 253-301.	3.3	16
150	Fe-decorated all-boron B40 fullerene serving as a potential promising active catalyst for CO oxidation: A DFT mechanistic approach. Polyhedron, 2020, 188, 114699.	2.2	16
151	Halogen bonds enhanced by Ïƒ-hole and Ï€-hole interactions: a comparative study on cooperativity and competition effects between Xâ˘™â˘™â˘™N and Sâ˘™â˘™â˘™N interactions in H3Nâ˘™â˘™â˘™XCNâ˘™â˘™â˘™SF2 and H3Nâ˘™â˘™â˘™	2.8	16
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