Mahdi D Esrafili

List of Publications by Year
in descending order

339	6,435	93792	206121
papers	citations	39 h-index	51 g-index

344	344	344	4034
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	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.	1.9	23
2	A DFT investigation into the effects of As-doping on the electronic structure and electrochemical activity of pyrite (FeS2). Journal of Molecular Graphics and Modelling, 2022, 110, 108040.	1.3	7
3	Coating all-boron B₃₈ fullerene with Ca and Al atoms for enhancing CO₂ capture: a DFT study. Molecular Physics, 2022, 120, .	0.8	2
4	The influence of Ag+ cation on elemental sulfur passive layer and adsorption behavior of chalcopyrite toward Fe3+ and Fe2+ ions: Insights from DFT calculations and molecular dynamics simulations. Physica B: Condensed Matter, 2022, 627, 413611.	1.3	2
5	Sc-functionalized porphyrin-like porous fullerene for CO2 storage and separation: A first-principles evaluation. Journal of Molecular Graphics and Modelling, 2022, 111, 108112.	1.3	3
6	Defect stabilized Fe atom on porous BN sheet as a potential electrocatalyst for oxygen reduction reaction: A first-principles investigation. Applied Surface Science, 2022, 580, 152271.	3.1	6
7	Co Anchored B 36 Cluster as a Novel Single Atom Catalyst for Removing Toxic CO Molecules: A Mechanistic Firstâ€Principles Study. ChemistrySelect, 2022, 7, .	0.7	2
8	Alkali metal decorated C₆₀ fullerenes as promising materials for delivery of the 5-fluorouracil anticancer drug: a DFT approach. RSC Advances, 2022, 12, 3948-3956.	1.7	15
9	Electrochemical reduction of NO catalyzed by boron-doped C₆₀ fullerene: a first-principles study. RSC Advances, 2022, 12, 3003-3012.	1.7	7
10	Carbon dioxide storage and separation using all-boron B38 fullerene: DFT calculations. Chemical Physics Letters, 2022, 790, 139361.	1.2	5
11	Y decorated all-boron B38 nanocluster for reversible molecular hydrogen storage: A first-principles investigation. International Journal of Hydrogen Energy, 2022, 47, 11611-11621.	3.8	7
12	NO adsorption on Ni4M (Mâ€‰=â€‰Ni, Mo, Sc, and Y) nanoclusters: a DFT study. Journal of Nanoparticle Research, 2022, 24, 1.	0.8	1
13	Ca functionalized N-doped porphyrin-like porous C60 as an efficient material for storage of molecular hydrogen. Journal of Molecular Modeling, 2022, 28, 20.	0.8	6
14	Systematic study of cooperative interplay between single-electron pnicogen bond and halogen bond in X₃CÂ·Â·Â·PH₂YÂ·Â·Â·ClY (X=H, CH₃; Y=CN, NC) complexes in two different minima configuration. Molecular Physics, 2022, 120, .	0.8	1
15	<scp>CO</scp> oxidation mediated by Alâ€doped <scp>ZnO</scp> nanoclusters: A firstâ€principles investigation. International Journal of Quantum Chemistry, 2022, 122, .	1.0	6
16	Silicon-doped boron nitride graphyne-like sheet for catalytic N2O reduction: A DFT study. Journal of Molecular Graphics and Modelling, 2022, 114, 108186.	1.3	3
17	Al- and Ga-embedded boron nitride nanotubes as effective nanocarriers for delivery of rizatriptan. Journal of Molecular Liquids, 2022, 361, 119662.	2.3	6
18	A computational study of CH4 storage on Sc functionalized C48B12 heterofullerene. Chemical Physics Letters, 2022, 802, 139751.	1.2	1

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19	DFT study of ferric ion interaction with passive layer on chalcopyrite surface: Elemental sulfur, defective sulfur and replacement of M2+(M=Cu and Fe) ions. Computational Condensed Matter, 2021, 26, e00536.	0.9	5
20	NO electrochemical reduction over Si-N4 embedded graphene: A DFT investigation. Applied Surface Science, 2021, 544, 148869.	3.1	24
21	A mechanistic first-principles study on N2 reduction reaction catalyzed by Ni4 supported defective graphene. Journal of Molecular Graphics and Modelling, 2021, 105, 107890.	1.3	1
22	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.	1.3	39
23	Catalytic role of B atoms in CO oxidation on B-doped graphene. Chemical Physics Letters, 2021, 776, 138714.	1.2	1
24	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.	6.5	27
25	Epoxidation of ethylene over an Ag atom embedded B-vacancy defective boron-nitride nanosheet via a trimolecular Langmuirâ€“Hinshelwood mechanism: A DFT investigation. Molecular Catalysis, 2021, 514, 111843.	1.0	1
26	DFT study and electrochemical investigation of Fe3+ion interaction on chalcopyrite (0 0 1)-S and M (MÂ=ÂCu, Fe) surfaces: A thermodynamic insights. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2021, 271, 115243.	1.7	3
27	Al-decorated C24N24 fullerene: A robust single-atom catalyst for CO oxidation. Polyhedron, 2021, , 115497.	1.0	5
28	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.	2.3	28
29	Ca coated B40 fullerene: A promising material for CO2 storage and separation. Chemical Physics Letters, 2021, 781, 138991.	1.2	9
30	Y-shape structured azo dyes with self-transforming feature to zwitterionic form as sensitizer for DSSC and DFT investigation of their photophysical and charge transfer properties. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 261, 120062.	2.0	6
31	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.	2.3	20
32	Catalytic CO oxidation reaction over N-substituted graphene nanoribbon with edge defects. Journal of Molecular Graphics and Modelling, 2021, 108, 108006.	1.3	3
33	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.	2.3	24
34	Single Al atom anchored on defective MoS2: An efficient catalytic site for reduction of greenhouse N2O gas by CO or C2H4 molecules. Applied Surface Science, 2021, 569, 151001.	3.1	6
35	Catalytic role of graphitic nitrogen atoms in the CO oxidation reaction over N-containing graphene: a first-principles mechanistic evaluation. New Journal of Chemistry, 2021, 45, 13822-13832.	1.4	1
36	Activation of the methane Câ€“H bond by Al- and Ga-doped graphenes: a DFT investigation. New Journal of Chemistry, 2021, 45, 19842-19851.	1.4	2

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37	Synergic effects between boron and nitrogen atoms in BN-codoped C_{59â^'n}BN_nfullerenes (n= 1â€“3) for metal-free reduction of greenhouse N₂O gas. RSC Advances, 2021, 11, 22598-22610.	1.7	9
38	Reversible CO2 storage and efficient separation using Ca decorated porphyrin-like porous C24N24 fullerene: a DFT study. RSC Advances, 2021, 11, 34402-34409.	1.7	4
39	A mechanistic DFT study of selective ethylene oxidation to ethylene oxide catalyzed by Pd-doped C3N monolayer. Surface Science, 2021, , 121981.	0.8	1
40	Efficient hydrogen storage on Al decorated C₂₄N₂₄: a DFT study. New Journal of Chemistry, 2021, 45, 21225-21235.	1.4	13
41	B-, N-doped and BN codoped C₆₀ heterofullerenes for environmental monitoring of NO and NO₂: a DFT study. Molecular Physics, 2020, 118, .	0.8	20
42	Constructing a dual-mode photochromic and intrinsically electrochromic device based on organic salts prepared by acid-base neutralization of pyromellitic diimides bearing a carboxyl group with aliphatic amines. Journal of Photochemistry and Photobiology A: Chemistry, 2020, 388, 112162.	2.0	8
43	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.	6.5	35
44	Development of TiO2 nanofibers based semiconducting humidity sensor: adsorption kinetics and DFT computations. Materials Chemistry and Physics, 2020, 239, 121981.	2.0	33
45	A comparative DFT study of Fe³⁺ and Fe²⁺ ions adsorption on (100) and (110) surfaces of pyrite: An electrochemical point of view. Surface and Interface Analysis, 2020, 52, 110-118.	0.8	10
46	Catalytic oxidation of CO using a silicon-coordinated carbon nitride fullerene. Molecular Physics, 2020, 118, .	0.8	10
47	Methane oxidation into methanol catalyzed by TM-anchored C24N24 nanoclusters (TMÂ=ÂFe, Co and Ni): A DFT study. Inorganic Chemistry Communication, 2020, 122, 108317.	1.8	14
48	Si-doped C₃N monolayers as efficient single-atom catalysts for the reduction of N₂O: a computational study. Molecular Physics, 2020, 118, e1759830.	0.8	1
49	Theoretical insights into oxygen reduction reaction catalyzed by phosphorus-doped divacancy C3N nanosheet. Journal of Molecular Graphics and Modelling, 2020, 100, 107647.	1.3	5
50	Fe-decorated all-boron B40 fullerene serving as a potential promising active catalyst for CO oxidation: A DFT mechanistic approach. Polyhedron, 2020, 188, 114699.	1.0	16
51	CuN3 doped graphene as an active electrocatalyst for oxygen reduction reaction in fuel cells: A DFT study. Journal of Molecular Graphics and Modelling, 2020, 96, 107537.	1.3	13
52	Tuning of pnicogen and chalcogen bonds by an aerogen-bonding interaction: a comparative ab initio study. Molecular Physics, 2019, 117, 58-66.	0.8	25
53	Interaction of ferric ion with (001)-S and (001)-M surfaces of chalcopyrite (Mâ€¯=â€¯Fe and Cu): Electrochemical insights from DFT calculations. Applied Surface Science, 2019, 495, 143529.	3.1	6
54	Catalytic reduction of N2O over Si-embedded MoS2 monolayer: A single-atom catalyst approach. Inorganic Chemistry Communication, 2019, 108, 107504.	1.8	8

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55	A promising and new single-atom catalyst for CO oxidation: Si-embedded MoS2 monolayer. Journal of Physics and Chemistry of Solids, 2019, 135, 109123.	1.9	14
56	Si-coordinated nitrogen doped graphene: A robust and highly active catalyst for NOâ€¯+â€¯CO reaction. Applied Surface Science, 2019, 494, 659-665.	3.1	9
57	Experimental and density functional theory study on humidity sensing properties of copper phthalocyanine (CuPc). Materials Research Express, 2019, 6, 105901.	0.8	4
58	Electrochemical Reduction of N₂ to NH₃ Using a Coâ€Atom Stabilized on Defective Nâ€Doped Graphene: A Computational Study. ChemistrySelect, 2019, 4, 12216-12226.	0.7	14
59	An effective approach for tuning catalytic activity of C3N nanosheets: Chemical-doping with the Si atom. Journal of Molecular Graphics and Modelling, 2019, 92, 320-328.	1.3	7
60	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.	2.9	16
61	Experimental and theoretical study of TiO2 based nanostructured semiconducting humidity sensor. Ceramics International, 2019, 45, 8362-8369.	2.3	39
62	Application of Novel Fe3O4â€“Polyaniline Nanocomposites in Asphaltene Adsorptive Removal: Equilibrium, Kinetic Study and DFT Calculations. Journal of Inorganic and Organometallic Polymers and Materials, 2019, 29, 1160-1170.	1.9	13
63	A computational study on the characteristics of open-shell H-bonding interaction between carbamic acid (NH2COOH) and HO2, HOS or HSO radicals. Journal of Molecular Modeling, 2019, 25, 189.	0.8	6
64	Computational mechanistic insights into CO oxidation reaction over Fe decorated C24N24 fullerene. Inorganic Chemistry Communication, 2019, 106, 190-196.	1.8	26
65	A comparative DFT study about surface reactivity and catalytic activity of Pd- and Ni-doped BN nanosheets: NO reduction by CO molecule. Structural Chemistry, 2019, 30, 1647-1657.	1.0	8
66	Electric field assisted activation of CO2 over P-doped graphene: A DFT study. Journal of Molecular Graphics and Modelling, 2019, 90, 192-198.	1.3	41
67	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.	1.6	42
68	C₅₉N Heterofullerene: A Promising Catalyst for NO Conversion into N₂O. ChemistrySelect, 2019, 4, 4308-4315.	0.7	6
69	B-doped C3N monolayer: a robust catalyst for oxidation of carbon monoxide. Theoretical Chemistry Accounts, 2019, 138, 1.	0.5	20
70	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.	1.3	22
71	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.	1.2	19
72	Catalytic reduction of nitrous oxide over boron-doped C3N monolayers: A DFT study. Chemical Physics Letters, 2019, 725, 52-58.	1.2	14

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73	C₅₉X Heterofullerenes (X=N, B, Si, P and S) as Catalysts for Reduction of N₂O: A Comparative DFT Study. ChemistrySelect, 2019, 4, 2267-2274.	0.7	12
74	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.	1.9	59
75	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.	0.9	43
76	CO catalytic oxidation over C59X heterofullerenes (Xâ€¯=â€¯B, Si, P, S): A DFT study. Computational and Theoretical Chemistry, 2019, 1151, 50-57.	1.1	11
77	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.	5.3	41
78	NO reduction over an Al-embedded MoS₂ monolayer: a first-principles study. RSC Advances, 2019, 9, 38973-38981.	1.7	11
79	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.	3.1	76
80	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.	1.3	16
81	N2O reduction over a porous Si-decorated carbon nitride fullerene: A DFT study. Chemical Physics Letters, 2019, 716, 11-16.	1.2	14
82	The influence of hydrogen- and lithium-bonding on the cooperativity of chalcogen bonds: A comparative ab initio study. Molecular Physics, 2019, 117, 726-733.	0.8	8
83	Graphene-Based Electrochemical Supercapacitors. Interface Science and Technology, 2019, 27, 339-386.	1.6	35
84	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.	3.1	63
85	The influence of halogen-bonding cooperativity on the hydrogen and lithium bonds: an ab initio study. Molecular Physics, 2019, 117, 1903-1911.	0.8	2
86	Adsorption sensitivity of pristine and Al- or Si-doped boron nitride nanoflake to COCl₂: a DFT study. Molecular Physics, 2019, 117, 626-634.	0.8	13
87	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.	1.0	17
88	Atomic Properties and Electronic Structure. Interface Science and Technology, 2019, , 23-66.	1.6	3
89	Oxygen Reduction Reaction. Interface Science and Technology, 2019, 27, 203-252.	1.6	15
90	Alcohol Oxidation and Hydrogen Evolution. Interface Science and Technology, 2019, 27, 253-301.	1.6	16

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91	Gas Convertor and Storage. Interface Science and Technology, 2019, 27, 387-437.	1.6	4
92	Synthesis and Surface Modification. Interface Science and Technology, 2019, 27, 67-108.	1.6	2
93	Al or Si decorated graphene-oxide: A promising material for capture and activation of ethylene and acetylene. Journal of Physics and Chemistry of Solids, 2018, 117, 42-48.	1.9	9
94	A computational study on the strength and nature of bifurcated aerogen bonds. Chemical Physics Letters, 2018, 698, 1-6.	1.2	17
95	Single Si atom supported on defective boron nitride nanosheet as a promising metalâ€free catalyst for N₂O reduction by CO or SO₂ molecule: A computational study. International Journal of Quantum Chemistry, 2018, 118, e25646.	1.0	6
96	Functional group effect of isoreticular metalâ€“organic frameworks on heavy metal ion adsorption. New Journal of Chemistry, 2018, 42, 8864-8873.	1.4	62
97	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.	1.3	16
98	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.	3.1	25
99	NO reduction by CO molecule over Si-doped boron nitride nanosheet: A dispersion-corrected DFT study. Chemical Physics Letters, 2018, 695, 131-137.	1.2	36
100	Metalâ€Free Reduction of NO over a Fullereneâ€like Boron Nitride Nanocluster: A Mechanistic Study by DFT Calculations. ChemistrySelect, 2018, 3, 1168-1175.	0.7	7
101	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.	1.3	49
102	CO Oxidation Catalyzed by a Single Ti Atom Supported on Divacancy Defective Graphene: A Dispersionâ€Corrected DFT Study. ChemistrySelect, 2018, 3, 4471-4479.	0.7	17
103	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.	3.1	39
104	N2Oâ€¯+â€¯CO reaction over single Ga or Ge atom embedded graphene: A DFT study. Surface Science, 2018, 667, 105-111.	0.8	12
105	Exploring hydride-Ï€ interactions and their tuning by Ïƒ-hole bonds: an ab initio study. Molecular Physics, 2018, 116, 118-128.	0.8	1
106	A catalyst-free achieving of N-doped carbon nanotubes: The healing of single-vacancy defects by NO molecule. Chemical Physics Letters, 2018, 691, 172-177.	1.2	4
107	Anionic tetrel bonds: An ab initio study. Chemical Physics Letters, 2018, 691, 394-400.	1.2	31
108	The strengthening effect of a halogen, chalcogen or pnicogen bonding on halogenâ€“Ï€ interaction: a comparative ab initio study. Molecular Physics, 2018, 116, 526-535.	0.8	6

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109	The triel bond: a potential force for tuning anionâ€“Ï€ interactions. Molecular Physics, 2018, 116, 388-398.	0.8	26
110	Chloropicrin sensor based on the pristine BN nanocones: DFT studies. Structural Chemistry, 2018, 29, 585-592.	1.0	11
111	Exploring Reaction Mechanisms for the Reduction of NO Molecules over Alâ€•or Siâ€Anchored Graphene Oxide: A Metalâ€Free Approach. ChemistrySelect, 2018, 3, 12072-12079.	0.7	4
112	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.	1.3	16
113	Strong Tetrel Bonds: Theoretical Aspects and Experimental Evidence. Molecules, 2018, 23, 2642.	1.7	43
114	Adsorptive mercaptan removal of liquid phase using nanoporous graphene: Equilibrium, kinetic study and DFT calculations. Ecotoxicology and Environmental Safety, 2018, 165, 533-539.	2.9	24
115	Epoxidation of ethylene over carbon and silicon-doped boron nitride sheets: A comparative DFT study. Solid State Communications, 2018, 284-286, 35-39.	0.9	10
116	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.	1.2	26
117	A DFT Study of Singleâ€Atom Catalysis of CO Oxidation Using Carbonâ€Embedded Hexagonal Boron Nitride Monolayer. ChemistrySelect, 2018, 3, 7402-7409.	0.7	15
118	N2Oâ€¯+â€¯CO reaction over a single Si or P atom incorporated nitrogen-doped graphene: A comparative DFT study. Chemical Physics Letters, 2018, 708, 94-99.	1.2	12
119	Carbon-doped boron-nitride fullerenes as efficient metal-free catalysts for oxidation of SO2: a DFT study. Structural Chemistry, 2018, 29, 275-283.	1.0	12
120	A Single Pd Atom Stabilized on Boronâ€Vacancy of hâ€BN Nanosheet: A Promising Catalyst for CO Oxidation. ChemistrySelect, 2018, 3, 9181-9188.	0.7	26
121	Boosting graphene reactivity with co-doping of boron and nitrogen atoms: CO oxidation by O2 molecule. Applied Surface Science, 2018, 455, 808-814.	3.1	40
122	Healing of a carbon-vacancy defect in silicon carbide nanotubes by CO molecules: A DFT study. Chemical Physics Letters, 2017, 671, 49-55.	1.2	8
123	An ab initio study on properties of cationic chalcogen bonds in XF₂Y⁺â¯NCZ (Xâ•H, CN, F; Yâ•S, Se; Zâ•H, Cl, Br) complexes. Journal of Sulfur Chemistry, 2017, 38, 83-97.	1.0	3
124	N2O + SO2 reaction over Si- and C-doped boron nitride nanotubes: A comparative DFT study. Applied Surface Science, 2017, 403, 43-50.	3.1	26
125	Cooperativity between the hydrogen bonding and Ïƒ-hole interaction in linear NCXÂ·Â·Â·(NCH)_n_{=2â€“5} and O₃ZÂ·Â·Â·(NCH)_n_{=2â€“5} complexes (X = Cl, Br; Z = Ar, Kr): a comparative study. Canadian Journal of Chemistry, 2017, 95, 537-546.	0.6	5
126	The effect of hydrogen-bonding cooperativity on the strength and properties of Ïƒ-hole interactions: an ab initio study. Molecular Physics, 2017, 115, 913-924.	0.8	14

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127	The enhancing effect of a cation-Ï€ interaction on the cooperativity of halogen bonds: A computational study. Journal of Molecular Graphics and Modelling, 2017, 73, 200-207.	1.3	3
128	A DFT study on the central-ring doped HBC nanographenes. Journal of Molecular Graphics and Modelling, 2017, 73, 101-107.	1.3	33
129	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.	2.1	16
130	A first-principles study on the adsorption behaviour of methanol and ethanol over C₅₉B heterofullerene. Molecular Physics, 2017, 115, 1633-1641.	0.8	19
131	Modulating of the pnicogen-bonding by a Hâ‹¯Ï€ interaction: An ab initio study. Journal of Molecular Graphics and Modelling, 2017, 75, 165-173.	1.3	13
132	Unusual cooperativity effects between halogen bond and donor-acceptor interactions: The role of orbital interaction. Chemical Physics Letters, 2017, 678, 275-282.	1.2	22
133	Chalcogen bonds tuned by an Nâ€“HÂ·Â·Â·Ï€ or Câ€“HÂ·Â·Â·Ï€ interaction: investigation of substituent, cooperativity and solvent effects. Molecular Physics, 2017, 115, 1713-1723.	0.8	12
134	A hard sphere fluid with quantum correction in nanospherical pores: A DFT study. Journal of Molecular Liquids, 2017, 238, 160-169.	2.3	2
135	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.	0.9	35
136	Mutual influence between triel bond and cationâ€“Ï€ interactions: an ab initio study. Molecular Physics, 2017, 115, 2999-3010.	0.8	10
137	Tuning aerogen bonds via anion-Ï€ or lone pair-Ï€ interaction: a comparative ab initio study. Structural Chemistry, 2017, 28, 1255-1264.	1.0	14
138	Carbeneâ€“aerogen bonds: an ab initio study. Molecular Physics, 2017, 115, 971-980.	0.8	13
139	A DFT study on catalytic epoxidation of ethylene over Ti-doped graphene nanoflake in the presence of NO molecules. Chemical Physics Letters, 2017, 687, 290-296.	1.2	10
140	Catalytic reduction of NO by CO molecules over Ni-doped graphene: a DFT investigation. New Journal of Chemistry, 2017, 41, 13149-13155.	1.4	23
141	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.	1.3	40
142	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.	1.4	16
143	Adsorption and decomposition of formaldehyde on the B12N12 nanostructure: a density functional theory study. Monatshefte FÃ¼r Chemie, 2017, 148, 1727-1731.	0.9	24
144	A DFT study on the healing of Nâ€vacancy defects in boron nitride nanosheets and nanotubes by a methylene molecule. International Journal of Quantum Chemistry, 2017, 117, e25450.	1.0	10

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145	A DFT study on the catalytic hydrogenation of CO2 to formic acid over Ti-doped graphene nanoflake. Chemical Physics Letters, 2017, 682, 49-54.	1.2	38
146	A structural study of fentanyl by DFT calculations, NMR and IR spectroscopy. Journal of Molecular Structure, 2017, 1128, 552-562.	1.8	38
147	A DFT study on electronic and optical properties of aspirin-functionalized B12N12 fullerene-like nanocluster. Structural Chemistry, 2017, 28, 735-748.	1.0	68
148	An ab initio study on anionic aerogen bonds. Chemical Physics Letters, 2017, 667, 337-344.	1.2	17
149	An ab initio study on substituent and cooperative effects in bifurcated fluorine bonds. Molecular Physics, 2017, 115, 278-287.	0.8	5
150	The Key Role of Orbital Interaction in Cooperativity between Bâ‹…â‹…â‹…N and Hydrogen/Lithium Bonding: An ab initio Study. ChemistrySelect, 2017, 2, 9113-9121.	0.7	1
151	Investigation of substituent effects in aerogenâ€bonding interaction between ZO₃ (Z=Kr,) Tj ETQq1 1 0.784314 rgBT /Ov	1.0	39
152	Microsolvation of CH+ in helium: An ab initio study. Journal of Theoretical and Computational Chemistry, 2016, 15, 1650018.	1.8	1
153	Oxidation of CO by N₂O over Al- and Ti-doped graphene: a comparative study. RSC Advances, 2016, 6, 64832-64840.	1.7	29
154	Symmetric bifurcated halogen bonds: substituent and cooperative effects. Molecular Physics, 2016, 114, 3610-3619.	0.8	4
155	The mutual influence of YÂ·Â·Â·N and HÂ·Â·Â·H interactions in XHYÂ·Â·Â·NCHÂ·Â·Â·HM complexes (X = F, Cl, Br; Y = S, Se;) Tj ETQq1 1 0.7 of Chemistry, 2016, 94, 567-573.	0.6	3
156	Ambient carbon dioxide capture by different dimensional AlN nanostructures: A comparative DFT study. Superlattices and Microstructures, 2016, 96, 164-173.	1.4	5
157	An ab initio study on the nature of Ï*f*-hole interactions in pnicogen-bonded complexes with carbene as an electron donor. Molecular Physics, 2016, 114, 2115-2122.	0.8	18
158	Insight into the intermolecular interactions in the NF₃â€“HSO system: a computational study. Journal of Sulfur Chemistry, 2016, 37, 674-682.	1.0	0
159	Substituent effects on geometry and bonding properties of asymmetric bifurcated pnicogen bonds: A theoretical study. Chemical Physics Letters, 2016, 650, 52-56.	1.2	9
160	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.	3.1	69
161	Exploring â€œaerogenâ€“hydrideâ€•interactions between ZOF2 (Z = Kr, Xe) and metal hydrides: An ab initio study. Chemical Physics Letters, 2016, 654, 23-28.	1.2	23
162	Tuning of tetrel bonds interactions by substitution and cooperative effects in XH₃SiÂ·Â·Â·NCHÂ·Â·Â·HM (X = H, F, Cl, Br; M = Li, Na, BeH and MgH) complexes. Molecular Physics, 2016, 114, 1974-1982.	0.8	9

#	Article	IF	Citations
163	Novel routes to quinoline derivatives from N-propargylamines. RSC Advances, 2016, 6, 49730-49746.	1.7	73
164	A comparative theoretical study of CO oxidation reaction by O2 molecule over Al- or Si-decorated graphene oxide. Journal of Molecular Graphics and Modelling, 2016, 69, 8-16.	1.3	10
165	Catalytic decomposition of hydrazine borane over pristine and Al-embedded boron nitride nanotubes: A DFT study. International Journal of Hydrogen Energy, 2016, 41, 20172-20184.	3.8	7
166	New route to 1,4-oxazepane and 1,4-diazepane derivatives: synthesis from N-propargylamines. RSC Advances, 2016, 6, 99781-99793.	1.7	48
167	A theoretical evidence for cooperative enhancement in aerogen-bonding interactions: Open-chain clusters of KrOF2 and XeOF2. Chemical Physics Letters, 2016, 662, 80-85.	1.2	36
168	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.	0.8	16
169	The healing of B- or N-vacancy defective BNNTs by using CO molecule: a DFT study. New Journal of Chemistry, 2016, 40, 8024-8031.	1.4	9
170	Single-electron aerogen bonds: Do they exist?. Chemical Physics Letters, 2016, 659, 196-202.	1.2	24
171	New page to access pyridine derivatives: synthesis from N-propargylamines. RSC Advances, 2016, 6, 71662-71675.	1.7	81
172	Halide ion-driven self-assembly of Zn(<scp>ii</scp>) compounds derived from an asymmetrical hydrazone building block: a combined experimental and theoretical study. New Journal of Chemistry, 2016, 40, 10116-10126.	1.4	11
173	Tuning of carbon bonds by substituent effects: an ab initio study. Molecular Physics, 2016, 114, 3658-3668.	0.8	9
174	Homonuclear chalcogenâ€“chalcogen bond interactions in complexes pairing <scp>YO</scp>₃ and <scp>YHX</scp> molecules (<scp>Yâ€‰=â€‰S, Se; Xâ€‰=â€‰H, Cl, Br, CCH, NC, OH) Tj ETQq0 Quantum Chemistry, 2016, 116, 529-536.	1.0	13
175	Competition between chalcogen bond and halogen bond interactions in YOX4:NH3 (YÂ=ÂS, Se; XÂ=ÂF, Cl, Br) complexes: An ab initio investigation. Structural Chemistry, 2016, 27, 1439-1447.	1.0	12
176	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.	0.8	22
177	A DFT study on the N₂O reduction by CO molecule over silicon carbide nanotubes and nanosheets. RSC Advances, 2016, 6, 59091-59099.	1.7	46
178	A DFT study on SO3 capture and activation over Si- or Al-doped graphene. Chemical Physics Letters, 2016, 658, 146-151.	1.2	28
179	Cooperativity in bifurcated lithium-bonded complexes: A DFT study. Chemical Physics Letters, 2016, 657, 195-198.	1.2	2
180	A density functional theory study on adsorption and decomposition of acetic acid over silicon carbide nanotubes. Synthetic Metals, 2016, 215, 164-169.	2.1	8

#	Article	IF	Citations
181	Al- or Si-decorated graphene oxide: A favorable metal-free catalyst for the N2O reduction. Applied Surface Science, 2016, 387, 454-460.	3.1	32
182	Strong cooperative effects between Ï€-hole and dihydrogen bonds interactions: a computational study. Molecular Physics, 2016, 114, 2315-2324.	0.8	10
183	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.	1.0	28
184	Catalytic activity of silicon carbide nanotubes and nanosheets for oxidation of CO: a DFT study. New Journal of Chemistry, 2016, 40, 2775-2784.	1.4	15
185	Pd-embedded graphene: An efficient and highly active catalyst for oxidation of CO. Superlattices and Microstructures, 2016, 92, 60-67.	1.4	50
186	Si-doped graphene: A promising metal-free catalyst for oxidation of SO2. Chemical Physics Letters, 2016, 649, 37-43.	1.2	57
187	A comparative study of the CO oxidation reaction over pristine and C-doped boron nitride fullerene. RSC Advances, 2016, 6, 17172-17178.	1.7	23
188	Cationic Pâ‹¯N interaction in XH 3 P + â‹¯NCY complexes (X = H, F, CN, NH 2 , OH; Y = H, Li, F, Cl) and its cooperativity with hydrogen/lithium/halogen bond. Journal of Molecular Graphics and Modelling, 2016, 64, 131-138.	1.3	5
189	Cooperativity of tetrel bonds tuned by substituent effects. Molecular Physics, 2016, 114, 1528-1538.	0.8	34
190	A novel multicomponent reaction between amino acids, aromatic aldehydes andp-toluenesulfonylmethyl isocyanide: an efficient and green one-pot synthesis using nanosilica. Green Chemistry Letters and Reviews, 2016, 9, 13-19.	2.1	5
191	Structural and photophysical characterization of mono- and binuclear Cu(<scp>i</scp>) complexes based on carbohydrazones: a combined experimental and computational study. CrystEngComm, 2016, 18, 2873-2884.	1.3	11
192	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	0.8	34
193	An ab initio study on cationic chalcogen bond interactions between F3â^'H S+ (n= 0â€“2) and nitrogen bases. Chemical Physics Letters, 2016, 645, 32-37.	1.2	11
194	Characterization of Ïƒ-hole interactions in 1:1 and 1:2 complexes of YOF2X (XÂ=ÂF, Cl, Br, I; YÂ=ÂP, As) with ammonia: competition between halogen and pnicogen bonds. Structural Chemistry, 2016, 27, 939-946.	1.0	11
195	Functionalization of single-walled (n,0) carbon and boron nitride nanotubes by carbonyl derivatives (n = 5, 6): a DFT study. Canadian Journal of Chemistry, 2016, 94, 105-111.	0.6	6
196	Chalcogen bonds formed through Ï€-holes: SO₃ complexes with nitrogen and phosphorus bases. Molecular Physics, 2016, 114, 276-282.	0.8	34
197	Strengthening halogenâ€¦â€‰halogen interactions by hydrogen and lithium bonds in NCMÂ·Â·Â·NCXÂ·Â·Â·YCH₃ and CNMÂ·Â·Â·CNXÂ·Â·Â·YCH₃ (M = H, Li and X,Y = Cl, Br) complexes: a comparative study. Molecular Physics, 2016, 114, 325-332.	0.8	8
198	Tuning tetrel bonds via cationâ€“Ï€ interactions: anab initiostudy on concerted interaction in M⁺â€“C₆H₅XH₃â€“NCY complexes (M = Li, Na, K; X = Si, Ge;) Tj ETQq0 0 0 rgBT /O	1.0	14

#	Article	IF	Citations
199	An ab initio investigation of chalcogenâ€“hydride interactions involving HXeH as a chalcogen bond acceptor. Structural Chemistry, 2016, 27, 785-792.	1.0	12
200	DFT calculations on the catalytic oxidation of CO over Si-doped (6,0) boron nitride nanotubes. Structural Chemistry, 2016, 27, 595-604.	1.0	27
201	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.	1.0	18
202	Chalcogenâ€“Chalcogen Interactions in Furan-YHX and Thiophene-YHX Complexes (X = F, Cl, Br; Y = S, Se): An Ab Initio Study. Bulletin of the Chemical Society of Japan, 2015, 88, 1683-1692.	2.0	5
203	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)	1.0	2
204	A Comparative Study of CO Oxidation on Nitrogenâ€•and PhosphorusâEDoped Graphene. ChemPhysChem, 2015, 16, 3719-3727.	1.0	70
205	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.	1.0	23
206	Cooperative effects between tetrel bond and other Ïƒâ€“hole bond interactions: a comparative investigation. Molecular Physics, 2015, 113, 3703-3711.	0.8	19
207	Cooperative and substitution effects in enhancing the strength of fluorine bonds by anionâ^Ï€ interactions. Canadian Journal of Chemistry, 2015, 93, 1169-1175.	0.6	3
208	Metal-Free Decomposition of Formic Acid on Pristine and Carbon-Doped Boron Nitride Fullerene: A DFT Study. Journal of Cluster Science, 2015, 26, 595-608.	1.7	11
209	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.	1.3	22
210	Experimental and theoretical study on diethyl-(Z)-2-(5,7-diphenyl-1,3,4-oxadiazepin-2-yl)-2-butenedioate using different levels of computational methods. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 140, 585-599.	2.0	12
211	Sensing and catalytic decomposition of hydrogen peroxide by silicon carbide nanotubes: A DFT study. International Journal of Quantum Chemistry, 2015, 115, 471-476.	1.0	6
212	Si-embedded boron-nitride nanotubes as an efficient and metal-free catalyst for NO oxidation. Superlattices and Microstructures, 2015, 81, 7-15.	1.4	26
213	Theoretical study on cooperative interplay between anionâ€“Ï€ and chalcogen-bonding interactions. Molecular Physics, 2015, 113, 1442-1450.	0.8	14
214	A DFT study of pyrazine derivatives and their Fe complexes in corrosion inhibition process. Journal of Molecular Structure, 2015, 1086, 64-72.	1.8	33
215	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.	0.8	18
216	Substituent effects in cooperativity of chalcogen bonds. Molecular Physics, 2015, 113, 3282-3290.	0.8	12

#	Article	IF	Citations
217	Does single-electron chalcogen bond exist? Some theoretical insights. Journal of Molecular Modeling, 2015, 21, 65.	0.8	41
218	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.	1.7	16
219	Sn-embedded graphene: An active catalyst for CO oxidation to CO 2 ?. Physica E: Low-Dimensional Systems and Nanostructures, 2015, 74, 382-387.	1.3	52
220	Bifurcated chalcogen bonds: A theoretical study on the structure, strength and bonding properties. Chemical Physics Letters, 2015, 634, 210-215.	1.2	52
221	Intrachain antiferromagnetic exchange in a 1D branched-chain built of two different copper(<scp>ii</scp>) centres interlinked by end-on azido and phenoxo bridges: electron density map, electrochemical and magnetic properties. RSC Advances, 2015, 5, 59926-59934.	1.7	14
222	An ab initio study on chalcogenâ€“chalcogen bond interactions in cyclic (SHX)3 complexes (X=F, Cl, CN,) Tj ETQq0 0 0 rgBT /Overlock 1	1.2	54
223	Prediction and characterisation of a chalcogenÂ·Â·Â·Ï€ interaction with acetylene as a potential electron donor in XHSÂ·Â·Â·HCCH and XHSeÂ·Â·Â·HCCH (X = F, Cl, Br, CN, OH, OCH₃, NH₂,) Tj ETQq1 1 0.784314 rg	0.8	8
224	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.	1.2	54
225	Theoretical study of formamide decomposition pathways over (6,0) silicon-carbide nanotube. Journal of Molecular Modeling, 2015, 21, 89.	0.8	2
226	Adsorption and decomposition of formamide over zigzag (n,0) silicon-carbide nanotubes (n = 5â€“7): Investigation of curvature effects. Surface Science, 2015, 637-638, 69-76.	0.8	14
227	The interaction energies between glycoluril clip and thiophenol derivatives using density functional theory calculations. Journal of Sulfur Chemistry, 2015, 36, 351-357.	1.0	7
228	Tuning of chalcogen bonds by cationâ€“Ï€ interactions: cooperative and diminutive effects. Journal of Molecular Modeling, 2015, 21, 300.	0.8	8
229	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.	1.1	19
230	Pnicogenâ€“pnicogen interactions in O2XP:PH2Y complexes (X=H, F, CN; Y=H, OH, OCH3, CH3, NH2). Chemical Physics Letters, 2015, 638, 122-127.	1.2	22
231	An ab initio study on tunability of Ï*f*-hole interactions in XHS:PH2Y and XH2P:SHY complexes (Xâ€‰=â€‰F, Cl, Br;) Tj ETQq1 1 0.78	0.8	20
232	Intriguing properties of unusual silicon nanocrystals. RSC Advances, 2015, 5, 78192-78208.	1.7	37
233	Can Si-embedded boron nitride nanotubes act as a favorable metal-free catalyst for CO oxidation by N₂O?. RSC Advances, 2015, 5, 100290-100298.	1.7	35
234	Supramolecular assemblies of organotin(<scp>iv</scp>)â€“diphosphoryl adducts: insights from X-rays and DFT. RSC Advances, 2015, 5, 98610-98617.	1.7	10

#	Article	IF	Citations
235	Catalytic decomposition of ammonia over silicon-carbide nanotube: a DFT study. Structural Chemistry, 2015, 26, 799-807.	1.0	7
236	Catalytic dehydrogenation of hydrazine on silicon-carbide nanotubes: A DFT study on the kinetic issue. Surface Science, 2015, 632, 118-125.	0.8	20
237	Hydrogen generation from methylamine using silicon carbide nanotubes as a dehydrogenation catalyst: A density functional theory study. Journal of Molecular Graphics and Modelling, 2015, 55, 41-47.	1.3	8
238	Effect of cationâ€“Ï€ interaction on lithium and halogen bonds: a comparative study. Molecular Physics, 2015, 113, 711-718.	0.8	10
239	Enhancement effect of lithium bonding on the strength ofÏ€-hole interactions in O₂SÂ·Â·Â·NCLiÂ·Â·Â·NCX and O₂SÂ·Â·Â·CNLiÂ·Â·Â·CNX complexes (X = H, F, CN, OH and) Tj ETQq1 1 0.784	0.8	3
240	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.	1.0	35
241	Carbon-Doped (6,0) Single-Walled Boron-Phosphide Nanotubes: A DFT Investigation of Electronic Structure, Surface Electrostatic Potential and QTAIM Analysis. Fullerenes Nanotubes and Carbon Nanostructures, 2015, 23, 142-147.	1.0	1
242	ÂA Computational Investigation Of Oxygen Reduction Reaction Mechanisms On Si- And Al-doped Graphene:ÂA Comparative Study. Advanced Materials Letters, 2015, 6, 527-530.	0.3	10
243	A DFT Study of Hydrogen Adsorption on Ln@B₁₆N₁₆Fullerene-Like Nanocage (Ln: La, Gd and Lu). Fullerenes Nanotubes and Carbon Nanostructures, 2014, 22, 928-937.	1.0	1
244	On the strength and nature of intermolecular XÂ·Â·Â·O interactions in CF2ClBrâ‹¯O3 complexes (X = F, Cl,) Tj ETQq0 0 0 rgBT /Overlock	0.6	7
245	A Computational Study of 1â€¯:â€¯1 and 1â€¯:â€¯2 Complexes of Naphthalene with Dimethyl Ether. Zeitschrift Fur Physikalische Chemie, 2014, 228, 115-125.	1.4	0
246	An ab initio study on the concerted interaction between chalcogen and pnicogen bonds. Journal of Molecular Modeling, 2014, 20, 2545.	0.8	18
247	A theoretical study of substitution effects on halogenâ€“Ï€ interactions. Molecular Physics, 2014, 112, 1160-1166.	0.8	44
248	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.	4.0	25
249	Exploring lithium bonding interactions between noble-gas hydrides HXeY and LiX molecules (Y=H, CN,) Tj ETQq1 1 0.784314 rgBT /Ov 2014, 1027, 84-90.	1.1	12
250	Theoretical study of the complementarity in halogenâ€“bonded complexes involving nitrogen and halogen as negative sites. Journal of Molecular Modeling, 2014, 20, 2101.	0.8	2
251	Characterization of halogenÂ·Â·Â·halogen interactions in crystalline dihalomethane compounds (CH2Cl2,) Tj ETQq1 1 0.784314 rgBT	0.8	7
252	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.	1.0	51

#	Article	IF	Citations
253	Synthesis, structural characterization and DFT calculations of a new one-dimensional diorganotin(IV) derivative of N-isonicotinyl phosphoramide. Polyhedron, 2014, 71, 8-16.	1.0	23
254	Mutual influence between conventional and unconventional lithium bonds. Journal of Molecular Graphics and Modelling, 2014, 49, 129-137.	1.3	7
255	Methylamine adsorption and decomposition on B12N12 nanocage: A density functional theory study. Surface Science, 2014, 626, 44-48.	0.8	61
256	A density functional theory study on the adsorption and decomposition of methanol on B12N12 fullerene-like nanocage. Superlattices and Microstructures, 2014, 67, 54-60.	1.4	67
257	Mutual interplay between pnicogen bond and dihydrogen bond in HMHâ‹¯HCNâ‹¯PH2X complexes (M=Be, Mg,) Tj ETQq1 1 0.784314	1.1	52
258	A theoretical insight into surface reactivity of nitrogen-doped BC3 nanotubes. Physica E: Low-Dimensional Systems and Nanostructures, 2014, 59, 223-229.	1.3	8
259	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.	0.8	20
260	Cooperative effects in hydrogen bond and pnicogen bond: a comparative study. Canadian Journal of Chemistry, 2014, 92, 1151-1156.	0.6	4
261	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.	0.8	18
262	A DFT study on the possibility of using boron nitride nanotubes as a dehydrogenation catalyst for methanol. Applied Surface Science, 2014, 314, 90-96.	3.1	37
263	Efficient dehydrogenation of formic acid using Al 12 N 12 nanocage: A DFT study. Superlattices and Microstructures, 2014, 75, 17-26.	1.4	19
264	A theoretical study on surface reactivity of fluorinated (n,0) and (n,n) carbon nanotubes (n = 3â€“6). Canadian Journal of Chemistry, 2014, 92, 299-304.	0.6	2
265	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.	0.8	24
266	Substituent effects on cooperativity of pnicogen bonds. Journal of Molecular Modeling, 2014, 20, 2436.	0.8	16
267	CNXeCl and CNXeBr species as halogen bond donors: a quantum chemical study on the structure, properties, and nature of halogenÂ·Â·Â·nitrogen interactions. Journal of Molecular Modeling, 2014, 20, 2203.	0.8	9
268	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˜SF2and H3Nâ˜â˜â˜	2.8	18
269	Synthesis of the glycoluril derivatives by the HZSM-5 nanozeolite as a catalyst. Green Chemistry Letters and Reviews, 2014, 7, 119-125.	2.1	10
270	Halogen bond interactions enhanced by sodium bonds â€” Theoretical evidence for cooperative and substitution effects in NCXÂ·Â·Â·NCNaÂ·Â·Â·NCY complexes (X = F, Cl, Br, I; Y = H, F, OH). Canadian Journal of Chemistry, 2014, 92, 653-658.	0.6	6

#	Article	IF	Citations
271	Cooperative effects in pnicogen bonding: (PH2F)2â€“7 and (PH2Cl)2â€“7 clusters. Chemical Physics Letters, 2014, 609, 37-41.	1.2	44
272	Interplay and competition between the lithium bonding and halogen bonding: R₃CÂ·Â·Â·XCNÂ·Â·Â·LiCN and R₃CÂ·Â·Â·LiCNÂ·Â·Â·XCN as a working model (R = H,) Tj ETQq0 0 0 rgBT /Overloc	1.2	32
273	A density functional study of silicon fullerene endohedral X@Si20F20 and exohedral X-Si20F20 (X=O2â^', S2â^', Se2â^') complexes. Physica E: Low-Dimensional Systems and Nanostructures, 2014, 56, 69-73.	1.3	2
274	Substituent effects on cooperativity between lithium bonds. International Journal of Quantum Chemistry, 2014, 114, 295-301.	1.0	16
275	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 ETQq1 1 0.784314	1.2	40
276	Potential of C-doped boron nitride fullerene as a catalyst for methanol dehydrogenation. Computational Materials Science, 2014, 92, 172-177.	1.4	55
277	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.	1.0	18
278	Electronic structure and surface reactivity of BC3 nanotubes from first-principle calculations. Structural Chemistry, 2014, 25, 187-195.	1.0	6
279	Halogen-Bond Interactions Enhanced by Charge-Assisted Hydrogen Bonds: An Ab Initio Study. Bulletin of the Chemical Society of Japan, 2014, 87, 882-889.	2.0	7
280	A DFT study on electronic structure and local reactivity descriptors of pristine and carbon-substituted AlN nanotubes. Canadian Journal of Chemistry, 2013, 91, 711-717.	0.6	3
281	One-pot synthesis, FT-IR and density functional method (DFT) studies on N-benzyl-N-ethyl-N-[5-nitro-2-(1,1,3,3-Tetramethylbutylamino)-1-benzofuran-3-yl]amine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 116, 65-73.	2.0	14
282	A theoretical investigation of the characteristics of hydrogen/halogen bonding interactions in dibromo-nitroaniline. Journal of Molecular Modeling, 2013, 19, 1417-1427.	0.8	39
283	The response of selected isomers of B80 buckyball toward NH3 adsorption: a density functional theory investigation. Structural Chemistry, 2013, 24, 1273-1279.	1.0	2
284	HRgCN and HRgNC as halogen bond acceptors (Rg=Kr and Xe): A theoretical study upon strength and nature of halogenâ‹¯nitrogen and halogenâ‹¯carbon interactions. Computational and Theoretical Chemistry, 2013, 1020, 1-6.	1.1	6
285	Toward understanding the role of water molecules in the uptake of nitrosyl hydride by sulfuric acid aerosols: A computational study. Computational and Theoretical Chemistry, 2013, 1017, 78-84.	1.1	2
286	Cooperative effects in cyclic LiCN and HCN clusters: A comparative study. Computational and Theoretical Chemistry, 2013, 1022, 115-120.	1.1	14
287	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.	0.8	18
288	Theoretical study of the interplay between halogen bond and lithiumâ€“Ïƒ interactions: Cooperative and diminutive effects. Chemical Physics Letters, 2013, 588, 47-50.	1.2	38

#	Article	IF	Citations
289	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.	0.8	18
290	Exploring surface reactivity of phosphorous-doped (6,0) and (4,4) BC3 nanotubes: a DFT study. Journal of Molecular Modeling, 2013, 19, 4877-4886.	0.8	8
291	Cooperativity between fluorine-centered halogen bonds: investigation of substituent effects. Journal of Molecular Modeling, 2013, 19, 5625-5632.	0.8	7
292	Nitrogen-doping improves surface reactivity of carbon nanocone. Superlattices and Microstructures, 2013, 62, 140-148.	1.4	3
293	Investigation into the nature of interactions in aspirinâ€“water clusters including SAPT, AIM and NBO theories. Molecular Simulation, 2013, 39, 629-639.	0.9	6
294	Characteristics and nature of the halogen-bonding interactions between CCl₃F and ozone: a supermolecular and SAPT study. Molecular Physics, 2013, 111, 3770-3778.	0.8	4
295	Nitrogen-doped (6,0) carbon nanotubes: A comparative DFT study based on surface reactivity descriptors. Computational and Theoretical Chemistry, 2013, 1015, 1-7.	1.1	59
296	A DFT study on carbon-doping at different sites of (8, 0) boron nitride nanotube. Structural Chemistry, 2013, 24, 573-581.	1.0	41
297	A comparative study on carbon/silicon doping effects on electronic structure and surface electrostatic potential of (6,0) boron-nitride nanotube: a DFT investigation. Structural Chemistry, 2013, 24, 1207-1214.	1.0	10
298	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.	0.8	40
299	A DFT investigation on hydrogen- and halogen-bonding interactions in dichloroacetic acid: application of NMR-GIAO and Bader theories. Structural Chemistry, 2013, 24, 39-47.	1.0	11
300	A quantum chemistry study on surface reactivity of pristine and carbon-substituted AlN nanotubes. Physica E: Low-Dimensional Systems and Nanostructures, 2013, 53, 161-167.	1.3	4
301	Revealing substitution effects on the strength and nature of halogen-hydride interactions: a theoretical study. Journal of Molecular Modeling, 2013, 19, 3767-3777.	0.8	45
302	Nitrogen-doped (6,0) and (4,4) single-walled SiC nanotubes: A DFT study on surface reactivity and NMR parameters. Superlattices and Microstructures, 2013, 60, 179-191.	1.4	9
303	Influence of oxygen/sulfur-termination on electronic structure and surface electrostatic potential of (6,0) carbon nanotube: a DFT study. Structural Chemistry, 2013, 24, 1571-1578.	1.0	8
304	Insights into the strength and nature of carbeneÂ·Â·Â·halogen bond interactions: a theoretical perspective. Journal of Molecular Modeling, 2013, 19, 2559-2566.	0.8	63
305	Theoretical insight into cooperativity in lithium-bonded complexes: Linear clusters of LiCN and LiNC. Chemical Physics Letters, 2013, 577, 6-10.	1.2	40
306	A DFT INVESTIGATION ON BASIS SET SIZE AND HYDROGEN-BONDING EFFECTS ON 17O AND 2H NQR PARAMETERS. Journal of Theoretical and Computational Chemistry, 2013, 12, 1350022.	1.8	1

#	Article	IF	Citations
307	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.	0.8	55
308	Symmetry-adapted perturbation theory study for some magnesium complexes. Canadian Journal of Chemistry, 2012, 90, 819-827.	0.6	0
309	A theoretical study on H-bonding interactions in maleic acid: calculated¹⁷O,¹H NMR parameters and QTAIM analysis. Molecular Simulation, 2012, 38, 896-905.	0.9	5
310	A theoretical study on bonding and energy aspects of and [LnL₃â€‰Â·â€‰H₂O]³⁺complexes (Lnâ€‰=â€‰La, Eu, Gd, Lâ€‰Â·â€‰	0.8	
311	A theoretical investigation on the nature of Clâ‹¯N and Brâ‹¯N halogen bonds in FArXâ‹¯NCY complexes (X=Cl,) Tj ETQq1 1 0.784314 r	1.1	56
312	A theoretical investigation on geometry and electronic structure of small FemSn nanoclusters (1â©½m,nâ©½4). Computational and Theoretical Chemistry, 2012, 1001, 1-6.	1.1	8
313	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.	1.6	35
314	Characterization of intermolecular interactions in crystalline aspirin: A computational NQR study. International Journal of Quantum Chemistry, 2012, 112, 1392-1400.	1.0	4
315	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.	0.8	42
316	DFT study of 17O, 1H and 13C NMR chemical shifts in two forms of native cellulose, I and I. Carbohydrate Research, 2012, 347, 99-106.	1.1	12
317	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.	0.8	66
318	Intra- and inter-molecular interactions in salicylic acid â€" Theoretical calculations of ¹⁷O and ¹H chemical shielding tensors and QTAIM analysis. Canadian Journal of Chemistry, 2011, 89, 1410-1418.	0.6	5
319	Characterization of Oâ€"Hâ‹¯O interactions in linear and cyclic clusters of boric acid: An ab initio, DFT, QTAIM and NBO study. Computational and Theoretical Chemistry, 2011, 974, 66-75.	1.1	7
320	A theoretical investigation of hydrogen bonding effects on oxygen and hydrogen chemical shielding tensors of aspirin. Structural Chemistry, 2011, 22, 1195-1203.	1.0	8
321	Computational study on the characteristics of the interaction in linear urea clusters. International Journal of Quantum Chemistry, 2011, 111, 3184-3195.	1.0	39
322	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.	0.5	21
323	A computational study of water adsorption on boron nitride nanotube. Structural Chemistry, 2010, 21, 903-908.	1.0	33
324	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.	1.3	37

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325	Structures and bonding patterns of nanoannular carbon clusters (C4â€“C20) through AIM analyses. Structural Chemistry, 2009, 20, 839-846.	1.0	5
326	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.	1.3	37
327	A density functional study of 15N chemical shielding tensors in quinolines. Chemical Physics Letters, 2009, 476, 196-200.	1.2	7
328	Characterization of cooperative effects in linear Î±-glycylglycine clusters. Biophysical Chemistry, 2009, 143, 26-33.	1.5	7
329	15N CHEMICAL SHIFT CALCULATIONS AND NATURAL BONDING ORBITAL ANALYSES OF (BENZAMIDE)n = 1 - 6 CLUSTERS. Journal of Theoretical and Computational Chemistry, 2009, 08, 973-982.	1.8	3
330	Theoretical 14N nuclear quadrupole resonance parameters for sulfa drugs: Sulfamerazine and sulfathiazole. Journal of Molecular Graphics and Modelling, 2008, 27, 326-331.	1.3	31
331	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.	1.5	28
332	A theoretical study of repeating sequence in HRP II: A combination of molecular dynamics simulations and 17O quadrupole coupling tensors. Biophysical Chemistry, 2008, 137, 76-80.	1.5	1
333	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.	0.5	50
334	Role of spin state on the geometry and nuclear quadrupole resonance parameters in hemin complex. Biophysical Chemistry, 2008, 134, 200-206.	1.5	3
335	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.	0.9	32
336	DENSITY FUNCTIONAL THEORY STUDY OF BINDING ENERGIES, 7Li NUCLEAR MAGNETIC SHIELDING, AND ELECTRIC FIELD GRADIENT TENSORS ON THE SMALL CLUSTERS OF LinHm (m â‰¤ n â‰¤ 4). Journal of Theoretical and Computational Chemistry, 2007, 06, 959-973.	1.8	4
337	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.	1.1	38
338	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.	1.5	35
339	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.	0.9	30