Mahdi D Esrafili

List of Publications by Year in Descending Order

332 papers	5,083 citations	36 h-index	46 g-index
344 ext. papers	5,819 ext. citations	2.7 avg, IF	6.95 L-index

#	Paper	IF	Citations
332	Alkali metal decorated C fullerenes as promising materials for delivery of the 5-fluorouracil anticancer drug: a DFT approach.. *RSC Advances*, **2022**, 12, 3948-3956	3.7	2
331	Electrochemical reduction of NO catalyzed by boron-doped C fullerene: a first-principles study.. *RSC Advances*, **2022**, 12, 3003-3012	3.7	1
330	Carbon dioxide storage and separation using all-boron B38 fullerene: DFT calculations. *Chemical Physics Letters*, **2022**, 790, 139361	2.5	0
329	Y decorated all-boron B38 nanocluster for reversible molecular hydrogen storage: A first-principles investigation. *International Journal of Hydrogen Energy*, **2022**,	6.7	1
328	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	2.8	0
327	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	6.7	0
326	A DFT investigation into the effects of As-doping on the electronic structure and electrochemical activity of pyrite (FeS). *Journal of Molecular Graphics and Modelling*, **2022**, 110, 108040	2.8	0
325	NO adsorption on Ni4M (M = Ni, Mo, Sc, and Y) nanoclusters: a DFT study. *Journal of Nanoparticle Research*, **2022**, 24, 1	2.3	
324	Silicon-doped boron nitride graphyne-like sheet for catalytic NO reduction: A DFT study.. *Journal of Molecular Graphics and Modelling*, **2022**, 114, 108186	2.8	1
323	Efficient hydrogen storage on Al decorated C24N24: a DFT study. *New Journal of Chemistry*, **2021**, 45, 21225-21235	3.6	0
322	Sc-functionalized porphyrin-like porous fullerene for CO storage and separation: A first-principles evaluation.. *Journal of Molecular Graphics and Modelling*, **2021**, 111, 108112	2.8	0
321	Reversible CO storage and efficient separation using Ca decorated porphyrin-like porous CN fullerene: a DFT study.. *RSC Advances*, **2021**, 11, 34402-34409	3.7	0
320	A mechanistic DFT study of selective ethylene oxidation to ethylene oxide catalyzed by Pd-doped C3N monolayer. *Surface Science*, **2021**, 121981	1.8	0
319	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	1.7	3
318	NO electrochemical reduction over Si-N4 embedded graphene: A DFT investigation. *Applied Surface Science*, **2021**, 544, 148869	6.7	9
317	A mechanistic first-principles study on N reduction reaction catalyzed by Ni supported defective graphene. *Journal of Molecular Graphics and Modelling*, **2021**, 105, 107890	2.8	1
316	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	2.8	16

315	Catalytic role of B atoms in CO oxidation on B-doped graphene. *Chemical Physics Letters*, **2021**, 776, 138714	2.4	0
314	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	12.8	6
313	Epoxidation of ethylene over an Ag atom embedded B-vacancy defective boron-nitride nanosheet via a trimolecular Langmuir Hinshelwood mechanism: A DFT investigation. *Molecular Catalysis*, **2021**, 514, 111843	3.3	0
312	Optical and photocatalytic characteristics of Al and Cu doped TiO2: Experimental assessments and DFT calculations. *Journal of Physics and Chemistry of Solids*, **2021**, 161, 110404	3.9	2
311	DFT study and electrochemical investigation of Fe3+ion interaction on chalcopyrite (0 0 1)-S and M (M Cu, Fe) surfaces: A thermodynamic insights. *Materials Science and Engineering B: Solid-State Materials for Advanced Technology*, **2021**, 271, 115243	3.1	1
310	Al-decorated C24N24 fullerene: A robust single-atom catalyst for CO oxidation. *Polyhedron*, **2021**, 115492	2.7	0
309	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	6	10
308	Ca coated B40 fullerene: A promising material for CO2 storage and separation. *Chemical Physics Letters*, **2021**, 781, 138991	2.5	2
307	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	4.4	0
306	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	6	3
305	Catalytic CO oxidation reaction over N-substituted graphene nanoribbon with edge defects. *Journal of Molecular Graphics and Modelling*, **2021**, 108, 108006	2.8	1
304	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	6	7
303	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	6.7	4
302	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	3.6	0
301	Synergic effects between boron and nitrogen atoms in BN-codoped C BN fullerenes (= 1-3) for metal-free reduction of greenhouse NO gas.. *RSC Advances*, **2021**, 11, 22598-22610	3.7	6
300	Ca functionalized N-doped porphyrin-like porous C as an efficient material for storage of molecular hydrogen.. *Journal of Molecular Modeling*, **2021**, 28, 20	2	1
299	Si-doped C3N monolayers as efficient single-atom catalysts for the reduction of N2O: a computational study. *Molecular Physics*, **2020**, 118, e1759830	1.7	0
298	Theoretical insights into oxygen reduction reaction catalyzed by phosphorus-doped divacancy CN nanosheet. *Journal of Molecular Graphics and Modelling*, **2020**, 100, 107647	2.8	3

297	Fe-decorated all-boron B40 fullerene serving as a potential promising active catalyst for CO oxidation: A DFT mechanistic approach. *Polyhedron*, **2020**, 188, 114699	2.7	9
296	CuN 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	2.8	10
295	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	1.5	8
294	Catalytic oxidation of CO using a silicon-coordinated carbon nitride fullerene. *Molecular Physics*, **2020**, 118, e1797919	1.7	5
293	Methane oxidation into methanol catalyzed by TM-anchored C24N24 nanoclusters (TM□=□Fe, Co and Ni): A DFT study. *Inorganic Chemistry Communication*, **2020**, 122, 108317	3.1	5
292	B-, N-doped and BN codoped C60 heterofullerenes for environmental monitoring of NO and NO2: a DFT study. *Molecular Physics*, **2020**, 118, e1631495	1.7	13
291	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	4.7	5
290	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	12.8	21
289	Development of TiO2 nanofibers based semiconducting humidity sensor: adsorption kinetics and DFT computations. *Materials Chemistry and Physics*, **2020**, 239, 121981	4.4	12
288	An effective approach for tuning catalytic activity of CN nanosheets: Chemical-doping with the Si atom. *Journal of Molecular Graphics and Modelling*, **2019**, 92, 320-328	2.8	4
287	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	7	10
286	Experimental and theoretical study of TiO2 based nanostructured semiconducting humidity sensor. *Ceramics International*, **2019**, 45, 8362-8369	5.1	23
285	Application of Novel Fe3O4□Polyaniline Nanocomposites in Asphaltene Adsorptive Removal: Equilibrium, Kinetic Study and DFT Calculations. *Journal of Inorganic and Organometallic Polymers and Materials*, **2019**, 29, 1160-1170	3.2	8
284	A computational study on the characteristics of open-shell H-bonding interaction between carbamic acid (NHCOOH) and HO, HOS or HSO radicals. *Journal of Molecular Modeling*, **2019**, 25, 189	2	4
283	Computational mechanistic insights into CO oxidation reaction over Fe decorated C24N24 fullerene. *Inorganic Chemistry Communication*, **2019**, 106, 190-196	3.1	16
282	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	1.8	5
281	Electric field assisted activation of CO over P-doped graphene: A DFT study. *Journal of Molecular Graphics and Modelling*, **2019**, 90, 192-198	2.8	22
280	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	3.7	15

279	C59N Heterofullerene: A Promising Catalyst for NO Conversion into N2O. *ChemistrySelect*, **2019**, 4, 4308-4315	1.8	5
278	B-doped C3N monolayer: a robust catalyst for oxidation of carbon monoxide. *Theoretical Chemistry Accounts*, **2019**, 138, 1	1.9	15
277	A DFT study on NO reduction to NO using Al- and P-doped hexagonal boron nitride nanosheets. *Journal of Molecular Graphics and Modelling*, **2019**, 89, 41-49	2.8	13
276	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	2.5	14
275	Catalytic reduction of nitrous oxide over boron-doped C3N monolayers: A DFT study. *Chemical Physics Letters*, **2019**, 725, 52-58	2.5	9
274	C59X Heterofullerenes (X=N, B, Si, P and S) as Catalysts for Reduction of N2O: A Comparative DFT Study. *ChemistrySelect*, **2019**, 4, 2267-2274	1.8	10
273	Tuning of pnicogen and chalcogen bonds by an aerogen-bonding interaction: a comparative ab initio study. *Molecular Physics*, **2019**, 117, 58-66	1.7	23
272	Interaction of ferric ion with (001)-S and (001)-M surfaces of chalcopyrite (M = Fe and Cu): Electrochemical insights from DFT calculations. *Applied Surface Science*, **2019**, 495, 143529	6.7	4
271	Catalytic reduction of N2O over Si-embedded MoS2 monolayer: A single-atom catalyst approach. *Inorganic Chemistry Communication*, **2019**, 108, 107504	3.1	6
270	A promising and new single-atom catalyst for CO oxidation: Si-embedded MoS2 monolayer. *Journal of Physics and Chemistry of Solids*, **2019**, 135, 109123	3.9	11
269	Si-coordinated nitrogen doped graphene: A robust and highly active catalyst for NO + CO reaction. *Applied Surface Science*, **2019**, 494, 659-665	6.7	6
268	Experimental and density functional theory study on humidity sensing properties of copper phthalocyanine (CuPc). *Materials Research Express*, **2019**, 6, 105901	1.7	2
267	Electrochemical Reduction of N2 to NH3 Using a Co-Atom Stabilized on Defective N-Doped Graphene: A Computational Study. *ChemistrySelect*, **2019**, 4, 12216-12226	1.8	8
266	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	4.8	27
265	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	2.3	30
264	CO catalytic oxidation over C59X heterofullerenes (X = B, Si, P, S): A DFT study. *Computational and Theoretical Chemistry*, **2019**, 1151, 50-57	2	9
263	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	7.6	25
262	NO reduction over an Al-embedded MoS monolayer: a first-principles study.. *RSC Advances*, **2019**, 9, 38973-38981	3.7	41

261	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	6.7	56
260	Oxidation of SO over C-doped boron nitride nanosheets: The role of C-doping, and solvent effects. *Journal of Molecular Graphics and Modelling*, **2019**, 86, 209-218	2.8	9
259	N2O reduction over a porous Si-decorated carbon nitride fullerene: A DFT study. *Chemical Physics Letters*, **2019**, 716, 11-16	2.5	8
258	The influence of hydrogen- and lithium-bonding on the cooperativity of chalcogen bonds: A comparative ab initio study. *Molecular Physics*, **2019**, 117, 726-733	1.7	8
257	Graphene-Based Electrochemical Supercapacitors. *Interface Science and Technology*, **2019**, 27, 339-386	2.3	23
256	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	6.7	36
255	The influence of halogen-bonding cooperativity on the hydrogen and lithium bonds: an ab initio study. *Molecular Physics*, **2019**, 117, 1903-1911	1.7	1
254	Adsorption sensitivity of pristine and Al- or Si-doped boron nitride nanoflake to COCl2: a DFT study. *Molecular Physics*, **2019**, 117, 626-634	1.7	9
253	A DFT study on the possibility of using a single Cu atom incorporated nitrogen-doped graphene as a promising and highly active catalyst for oxidation of CO. *International Journal of Quantum Chemistry*, **2019**, 119, e25857	2.1	12
252	Atomic Properties and Electronic Structure. *Interface Science and Technology*, **2019**, 23-66	2.3	2
251	Oxygen Reduction Reaction. *Interface Science and Technology*, **2019**, 27, 203-252	2.3	8
250	Alcohol Oxidation and Hydrogen Evolution. *Interface Science and Technology*, **2019**, 27, 253-301	2.3	10
249	Gas Convertor and Storage. *Interface Science and Technology*, **2019**, 27, 387-437	2.3	2
248	Synthesis and Surface Modification. *Interface Science and Technology*, **2019**, 27, 67-108	2.3	1
247	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	3.9	6
246	A computational study on the strength and nature of bifurcated aerogen bonds. *Chemical Physics Letters*, **2018**, 698, 1-6	2.5	15
245	Single Si atom supported on defective boron nitride nanosheet as a promising metal-free catalyst for N2O reduction by CO or SO2 molecule: A computational study. *International Journal of Quantum Chemistry*, **2018**, 118, e25646	2.1	6
244	Functional group effect of isoreticular metal–organic frameworks on heavy metal ion adsorption. *New Journal of Chemistry*, **2018**, 42, 8864-8873	3.6	50

243	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	2.8	11
242	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	6.7	21
241	NO reduction by CO molecule over Si-doped boron nitride nanosheet: A dispersion-corrected DFT study. *Chemical Physics Letters*, **2018**, 695, 131-137	2.5	29
240	Metal-Free Reduction of NO over a Fullerene-like Boron Nitride Nanocluster: A Mechanistic Study by DFT Calculations. *ChemistrySelect*, **2018**, 3, 1168-1175	1.8	5
239	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	2.8	33
238	CO Oxidation Catalyzed by a Single Ti Atom Supported on Divacancy Defective Graphene: A Dispersion-Corrected DFT Study. *ChemistrySelect*, **2018**, 3, 4471-4479	1.8	15
237	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	6.7	28
236	N2O + CO reaction over single Ga or Ge atom embedded graphene: A DFT study. *Surface Science*, **2018**, 667, 105-111	1.8	7
235	Exploring hydride-π interactions and their tuning by π-hole bonds: an ab initio study. *Molecular Physics*, **2018**, 116, 118-128	1.7	1
234	N2O + CO reaction over a single Si or P atom incorporated nitrogen-doped graphene: A comparative DFT study. *Chemical Physics Letters*, **2018**, 708, 94-99	2.5	9
233	Carbon-doped boron-nitride fullerenes as efficient metal-free catalysts for oxidation of SO2: a DFT study. *Structural Chemistry*, **2018**, 29, 275-283	1.8	8
232	A Single Pd Atom Stabilized on Boron-Vacancy of h-BN Nanosheet: A Promising Catalyst for CO Oxidation. *ChemistrySelect*, **2018**, 3, 9181-9188	1.8	19
231	Boosting graphene reactivity with co-doping of boron and nitrogen atoms: CO oxidation by O2 molecule. *Applied Surface Science*, **2018**, 455, 808-814	6.7	27
230	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	2.5	4
229	Anionic tetrel bonds: An ab initio study. *Chemical Physics Letters*, **2018**, 691, 394-400	2.5	26
228	The strengthening effect of a halogen, chalcogen or pnicogen bonding on halogen-π interaction: a comparative ab initio study. *Molecular Physics*, **2018**, 116, 526-535	1.7	5
227	The triel bond: a potential force for tuning anion-π interactions. *Molecular Physics*, **2018**, 116, 388-398	1.7	20
226	Chloropicrin sensor based on the pristine BN nanocones: DFT studies. *Structural Chemistry*, **2018**, 29, 585-592	1.8	9

225	Exploring Reaction Mechanisms for the Reduction of NO Molecules over Al- or Si-Anchored Graphene Oxide: A Metal-Free Approach. *ChemistrySelect*, **2018**, 3, 12072-12079	1.8	2
224	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	2.8	12
223	Strong Tetrel Bonds: Theoretical Aspects and Experimental Evidence. *Molecules*, **2018**, 23,	4.8	30
222	Adsorptive mercaptan removal of liquid phase using nanoporous graphene: Equilibrium, kinetic study and DFT calculations. *Ecotoxicology and Environmental Safety*, **2018**, 165, 533-539	7	17
221	Epoxidation of ethylene over carbon and silicon-doped boron nitride sheets: A comparative DFT study. *Solid State Communications*, **2018**, 284-286, 35-39	1.6	6
220	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	2.5	20
219	A DFT Study of Single-Atom Catalysis of CO Oxidation Using Carbon-Embedded Hexagonal Boron Nitride Monolayer. *ChemistrySelect*, **2018**, 3, 7402-7409	1.8	10
218	Healing of a carbon-vacancy defect in silicon carbide nanotubes by CO molecules: A DFT study. *Chemical Physics Letters*, **2017**, 671, 49-55	2.5	7
217	An ab initio study on properties of cationic chalcogen bonds in XF2Y+?NCZ (X?H, CN, F; Y?S, Se; Z?H, Cl, Br) complexes. *Journal of Sulfur Chemistry*, **2017**, 38, 83-97	2.3	3
216	N2O + SO2 reaction over Si- and C-doped boron nitride nanotubes: A comparative DFT study. *Applied Surface Science*, **2017**, 403, 43-50	6.7	21
215	Cooperativity between the hydrogen bonding and □hole interaction in linear NCX□□(NCH)n=2□ and O3Z□□(NCH)n=2□ complexes (X = Cl, Br; Z = Ar, Kr): a comparative study. *Canadian Journal of Chemistry*, **2017**, 95, 537-546	0.9	5
214	The effect of hydrogen-bonding cooperativity on the strength and properties of □hole interactions: an ab initio study. *Molecular Physics*, **2017**, 115, 913-924	1.7	10
213	The enhancing effect of a cation-□interaction on the cooperativity of halogen bonds: A computational study. *Journal of Molecular Graphics and Modelling*, **2017**, 73, 200-207	2.8	0
212	A DFT study on the central-ring doped HBC nanographenes. *Journal of Molecular Graphics and Modelling*, **2017**, 73, 101-107	2.8	32
211	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	3.6	10
210	A first-principles study on the adsorption behaviour of methanol and ethanol over C59B heterofullerene. *Molecular Physics*, **2017**, 115, 1633-1641	1.7	14
209	Modulating of the pnicogen-bonding by a H?□nteraction: An ab initio study. *Journal of Molecular Graphics and Modelling*, **2017**, 75, 165-173	2.8	11
208	Unusual cooperativity effects between halogen bond and donor-acceptor interactions: The role of orbital interaction. *Chemical Physics Letters*, **2017**, 678, 275-282	2.5	15

207	Chalcogen bonds tuned by an NH⋯ or CH⋯ interaction: investigation of substituent, cooperativity and solvent effects. *Molecular Physics*, **2017**, 115, 1713-1723	1.7	11
206	A hard sphere fluid with quantum correction in nanospherical pores: A DFT study. *Journal of Molecular Liquids*, **2017**, 238, 160-169	6	2
205	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	2.3	30
204	Mutual influence between triel bond and cation⋯ interactions: an ab initio study. *Molecular Physics*, **2017**, 115, 2999-3010	1.7	8
203	Tuning aerogen bonds via anion- or lone pair- interaction: a comparative ab initio study. *Structural Chemistry*, **2017**, 28, 1255-1264	1.8	11
202	Carbene⋯aerogen bonds: an ab initio study. *Molecular Physics*, **2017**, 115, 971-980	1.7	9
201	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	2.5	6
200	Catalytic reduction of NO by CO molecules over Ni-doped graphene: a DFT investigation. *New Journal of Chemistry*, **2017**, 41, 13149-13155	3.6	17
199	Catalytic hydrogenation of CO over Pt- and Ni-doped graphene: A comparative DFT study. *Journal of Molecular Graphics and Modelling*, **2017**, 77, 143-152	2.8	29
198	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	3.6	12
197	Adsorption and decomposition of formaldehyde on the B12N12 nanostructure: a density functional theory study. *Monatshefte Für Chemie*, **2017**, 148, 1727-1731	1.4	16
196	A DFT study on the healing of N-vacancy defects in boron nitride nanosheets and nanotubes by a methylene molecule. *International Journal of Quantum Chemistry*, **2017**, 117, e25450	2.1	4
195	A DFT study on the catalytic hydrogenation of CO2 to formic acid over Ti-doped graphene nanoflake. *Chemical Physics Letters*, **2017**, 682, 49-54	2.5	27
194	A structural study of fentanyl by DFT calculations, NMR and IR spectroscopy. *Journal of Molecular Structure*, **2017**, 1128, 552-562	3.4	26
193	A DFT study on electronic and optical properties of aspirin-functionalized B12N12 fullerene-like nanocluster. *Structural Chemistry*, **2017**, 28, 735-748	1.8	53
192	An ab initio study on anionic aerogen bonds. *Chemical Physics Letters*, **2017**, 667, 337-344	2.5	15
191	An ab initio study on substituent and cooperative effects in bifurcated fluorine bonds. *Molecular Physics*, **2017**, 115, 278-287	1.7	4
190	The Key Role of Orbital Interaction in Cooperativity between B???N and Hydrogen/Lithium Bonding: An ab initio Study. *ChemistrySelect*, **2017**, 2, 9113-9121	1.8	1

189	An ab initio investigation of chalcogen–hydride interactions involving HXeH as a chalcogen bond acceptor. *Structural Chemistry*, **2016**, 27, 785-792	1.8	9
188	DFT calculations on the catalytic oxidation of CO over Si-doped (6,0) boron nitride nanotubes. *Structural Chemistry*, **2016**, 27, 595-604	1.8	24
187	Hole bond tunability in YO2X2:NH3 and YO2X2:H2O complexes (X = F, Cl, Br; Y = S, Se): trends and theoretical aspects. *Structural Chemistry*, **2016**, 27, 617-625	1.8	18
186	A theoretical evidence for cooperative enhancement in aerogen-bonding interactions: Open-chain clusters of KrOF2 and XeOF2. *Chemical Physics Letters*, **2016**, 662, 80-85	2.5	30
185	The strengthening effect of a hydrogen or lithium bond on the Z⋯N aerogen bond (Z = Ar, Kr and Xe): a comparative study. *Molecular Physics*, **2016**, 114, 3265-3276	1.7	15
184	The healing of B- or N-vacancy defective BNNTs by using CO molecule: a DFT study. *New Journal of Chemistry*, **2016**, 40, 8024-8031	3.6	7
183	Single-electron aerogen bonds: Do they exist?. *Chemical Physics Letters*, **2016**, 659, 196-202	2.5	22
182	New page to access pyridine derivatives: synthesis from N-propargylamines. *RSC Advances*, **2016**, 6, 71662-71676	3.7	16
181	Halide ion-driven self-assembly of Zn(II) compounds derived from an asymmetrical hydrazone building block: a combined experimental and theoretical study. *New Journal of Chemistry*, **2016**, 40, 10116-10126	3.6	11
180	Tuning of carbon bonds by substituent effects: an ab initio study. *Molecular Physics*, **2016**, 114, 3658-3668	1.7	9
179	Homonuclear chalcogen–chalcogen bond interactions in complexes pairing YO3 and YHX molecules (Y = S, Se; X = H, Cl, Br, CCH, NC, OH, OCH3): Influence of substitution and cooperativity. *International Journal of Quantum Chemistry*, **2016**, 116, 529-536	2.1	9
178	Competition between chalcogen bond and halogen bond interactions in YOX4:NH3 (Y = S, Se; X = F, Cl, Br) complexes: An ab initio investigation. *Structural Chemistry*, **2016**, 27, 1439-1447	1.8	10
177	Strengthening of the halogen-bonding by an aerogen bond interaction: substitution and cooperative effects in O3Z⋯NCX⋯NCY (Z = Ar, Kr, Xe; X = Cl, Br, I; Y = H, F, OH) complexes. *Molecular Physics*, **2016**, 114, 2177-2186	1.7	20
176	A DFT study on the N2O reduction by CO molecule over silicon carbide nanotubes and nanosheets. *RSC Advances*, **2016**, 6, 59091-59099	3.7	36
175	A DFT study on SO3 capture and activation over Si- or Al-doped graphene. *Chemical Physics Letters*, **2016**, 658, 146-151	2.5	16
174	Cooperativity in bifurcated lithium-bonded complexes: A DFT study. *Chemical Physics Letters*, **2016**, 657, 195-198	2.5	1
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