Mahdi D Esrafili

List of Publications by Citations

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	New page to access pyridine derivatives: synthesis from N-propargylamines. *RSC Advances*, **2016**, 6, 71662-71675	3.7	66
331	Novel routes to quinoline derivatives from N-propargylamines. *RSC Advances*, **2016**, 6, 49730-49746	3.7	66
330	Characteristics and nature of halogen bonds in linear clusters of NCX (X=Cl, and Br): an ab initio, NBO and QTAIM study. *Molecular Physics*, **2011**, 109, 2451-2460	1.7	65
329	A Comparative Study of CO Oxidation on Nitrogen- and Phosphorus-Doped Graphene. *ChemPhysChem*, **2015**, 16, 3719-27	3.2	64
328	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	6.7	62
327	A density functional theory study on the adsorption and decomposition of methanol on B12N12 fullerene-like nanocage. *Superlattices and Microstructures*, **2014**, 67, 54-60	2.8	60
326	A theoretical investigation on the nature of Cl?N and Br?N halogen bonds in FArX?NCY complexes (X = Cl, Br and Y = H, F, Cl, Br, OH, NH2, CH3 and CN). *Computational and Theoretical Chemistry*, **2012** , 997, 77-82	2	56
325	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
324	Insights into the strength and nature of carbene□halogen bond interactions: a theoretical perspective. *Journal of Molecular Modeling*, **2013**, 19, 2559-66	2	55
323	A DFT study on electronic and optical properties of aspirin-functionalized B12N12 fullerene-like nanocluster. *Structural Chemistry*, **2017**, 28, 735-748	1.8	53
322	Mutual interplay between pnicogen bond and dihydrogen bond in HMH?HCN?PH2X complexes (M = Be, Mg, Zn; X = H, F, Cl). *Computational and Theoretical Chemistry*, **2014**, 1034, 1-6	2	52
321	Potential of C-doped boron nitride fullerene as a catalyst for methanol dehydrogenation. *Computational Materials Science*, **2014**, 92, 172-177	3.2	52
320	An ab initio study on chalcogen□halcogen bond interactions in cyclic (SHX)3 complexes (X = F, Cl, CN, NC, CCH, OH, OCH3, NH2). *Chemical Physics Letters*, **2015**, 628, 71-75	2.5	51
319	Nitrogen-doped (6,0) carbon nanotubes: A comparative DFT study based on surface reactivity descriptors. *Computational and Theoretical Chemistry*, **2013**, 1015, 1-7	2	51
318	Functional group effect of isoreticular metal□rganic frameworks on heavy metal ion adsorption. *New Journal of Chemistry*, **2018**, 42, 8864-8873	3.6	50
317	A theoretical evidence for mutual influence between S□□N(C) and hydrogen/lithium/halogen bonds: competition and interplay between □hole and □hole interactions. *Structural Chemistry*, **2014**, 25, 1197-1205	1.8	50
316	Tetrel bond cooperativity in open-chain (CH3CN)n and (CH3NC)n clusters (n=2□): An ab initio study. *Chemical Physics Letters*, **2015**, 628, 16-20	2.5	49

315	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, 5005-16	2	49
314	Bifurcated chalcogen bonds: A theoretical study on the structure, strength and bonding properties. *Chemical Physics Letters*, **2015**, 634, 210-215	2.5	48
313	Sn-embedded graphene: An active catalyst for CO oxidation to CO 2 ?. *Physica E: Low-Dimensional Systems and Nanostructures*, **2015**, 74, 382-387	3	46
312	Pd-embedded graphene: An efficient and highly active catalyst for oxidation of CO. *Superlattices and Microstructures*, **2016**, 92, 60-67	2.8	46
311	Methylamine adsorption and decomposition on B12N12 nanocage: A density functional theory study. *Surface Science*, **2014**, 626, 44-48	1.8	45
310	New route to 1,4-oxazepane and 1,4-diazepane derivatives: synthesis from N-propargylamines. *RSC Advances*, **2016**, 6, 99781-99793	3.7	44
309	Theoretical study of NH□□□O hydrogen bonding properties and cooperativity effects in linear acetamide clusters. *Theoretical Chemistry Accounts*, **2008**, 121, 135-146	1.9	43
308	A theoretical study of substitution effects on halogen□interactions. *Molecular Physics*, **2014**, 112, 1160-1166	1.7	42
307	Revealing substitution effects on the strength and nature of halogen-hydride interactions: a theoretical study. *Journal of Molecular Modeling*, **2013**, 19, 3767-77	2	41
306	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, 2003-11	2	40
305	Does single-electron chalcogen bond exist? Some theoretical insights. *Journal of Molecular Modeling*, **2015**, 21, 65	2	39
304	Si-doped graphene: A promising metal-free catalyst for oxidation of SO2. *Chemical Physics Letters*, **2016**, 649, 37-43	2.5	39
303	Cooperative effects in pnicogen bonding: (PH2F)2□ and (PH2Cl)2□ clusters. *Chemical Physics Letters*, **2014**, 609, 37-41	2.5	39
302	A DFT study on carbon-doping at different sites of (8, 0) boron nitride nanotube. *Structural Chemistry*, **2013**, 24, 573-581	1.8	39
301	Cooperativity effects between □hole interactions: a theoretical evidence for mutual influence between chalcogen bond and halogen bond interactions in F2S□□NCX□□NCY complexes (X = F, Cl, Br, I; Y = H, F, OH). *Molecular Physics*, **2014**, 112, 2746-2752	1.7	38
300	A theoretical investigation of the characteristics of hydrogen/halogen bonding interactions in dibromo-nitroaniline. *Journal of Molecular Modeling*, **2013**, 19, 1417-27	2	38
299	Theoretical study of the interplay between halogen bond and lithium□interactions: Cooperative and diminutive effects. *Chemical Physics Letters*, **2013**, 588, 47-50	2.5	37
298	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

297	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, 2375-82	2	36
296	Computational study on the characteristics of the interaction in linear urea clusters. *International Journal of Quantum Chemistry*, **2011**, 111, 3184-3195	2.1	36
295	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, 963-70	2.8	36
294	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
293	Theoretical insight into cooperativity in lithium-bonded complexes: Linear clusters of LiCN and LiNC. *Chemical Physics Letters*, **2013**, 577, 6-10	2.5	35
292	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	3	35
291	A DFT study on the possibility of using boron nitride nanotubes as a dehydrogenation catalyst for methanol. *Applied Surface Science*, **2014**, 314, 90-96	6.7	34
290	Investigation of substituent effects in aerogen-bonding interaction between ZO3 (Z=Kr, Xe) and nitrogen bases. *International Journal of Quantum Chemistry*, **2016**, 116, 1254-1260	2.1	34
289	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
288	A computational study of water adsorption on boron nitride nanotube. *Structural Chemistry*, **2010**, 21, 903-908	1.8	33
287	A DFT study on the central-ring doped HBC nanographenes. *Journal of Molecular Graphics and Modelling*, **2017**, 73, 101-107	2.8	32
286	Can Si-embedded boron nitride nanotubes act as a favorable metal-free catalyst for CO oxidation by N2O?. *RSC Advances*, **2015**, 5, 100290-100298	3.7	32
285	Ab initio calculations of cooperativity effects on chalcogen bonding: linear clusters of (OCS)2 and (OCSe)2. *Structural Chemistry*, **2015**, 26, 199-206	1.8	32
284	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	2.8	32
283	Cooperativity of tetrel bonds tuned by substituent effects. *Molecular Physics*, **2016**, 114, 1528-1538	1.7	31
282	Influence of N-H...O and O-H...O hydrogen bonds on the (17)O, (15)N and (13)C chemical shielding tensors in crystalline acetaminophen: a density functional theory study. *Biophysical Chemistry*, **2007**, 128, 38-45	3.5	31
281	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
280	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

279	14N and 17O electric field gradient tensors in benzamide clusters: Theoretical evidence for cooperative and electronic delocalization effects in NH?O hydrogen bonding. *Chemical Physics*, **2008**, 348, 175-180	2.3	30
278	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
277	Strong Tetrel Bonds: Theoretical Aspects and Experimental Evidence. *Molecules*, **2018**, 23,	4.8	30
276	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
275	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
274	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, 1597-608	4.3	29
273	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	2.3	29
272	Theoretical 14N nuclear quadrupole resonance parameters for sulfa drugs: sulfamerazine and sulfathiazole. *Journal of Molecular Graphics and Modelling*, **2008**, 27, 326-31	2.8	29
271	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
270	Al- or Si-decorated graphene oxide: A favorable metal-free catalyst for the N2O reduction. *Applied Surface Science*, **2016**, 387, 454-460	6.7	28
269	Chalcogen bonds formed through holes: SO3 complexes with nitrogen and phosphorus bases. *Molecular Physics*, **2016**, 114, 276-282	1.7	28
268	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
267	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
266	Density functional theory study of N-H...O, O-H...O and C-H...O hydrogen-bonding effects on the 14N and 2H nuclear quadrupole coupling tensors of N-acetyl-valine. *Biophysical Chemistry*, **2008**, 133, 11-8	3.5	27
265	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
264	A structural study of fentanyl by DFT calculations, NMR and IR spectroscopy. *Journal of Molecular Structure*, **2017**, 1128, 552-562	3.4	26
263	A DFT study of pyrazine derivatives and their Fe complexes in corrosion inhibition process. *Journal of Molecular Structure*, **2015**, 1086, 64-72	3.4	26
262	Oxidation of CO by N2O over Al- and Ti-doped graphene: a comparative study. *RSC Advances*, **2016**, 6, 64832-64840	3.7	26

261	Anionic tetrel bonds: An ab initio study. *Chemical Physics Letters*, **2018**, 691, 394-400	2.5	26
260	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
259	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
258	Theoretical insights into nature of 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	1.8	24
257	Experimental and theoretical study of TiO2 based nanostructured semiconducting humidity sensor. *Ceramics International*, **2019**, 45, 8362-8369	5.1	23
256	Intriguing properties of unusual silicon nanocrystals. *RSC Advances*, **2015**, 5, 78192-78208	3.7	23
255	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
254	Enhancement effect of lithium bonding on the strength of pnicogen bonds: XH2P⋯NCLi⋯NCY as a working model (X = F, Cl; Y = H, F, Cl, CN). *Molecular Physics*, **2014**, 112, 2058-2062	1.7	23
253	Graphene-Based Electrochemical Supercapacitors. *Interface Science and Technology*, **2019**, 27, 339-386	2.3	23
252	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
251	Single-electron aerogen bonds: Do they exist?. *Chemical Physics Letters*, **2016**, 659, 196-202	2.5	22
250	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	2.1	22
249	Mutual influence between anion-and pnicogen bond interactions: the enhancement of P?N and P?O interactions by an anion-bond. *Journal of Molecular Graphics and Modelling*, **2015**, 57, 99-105	2.8	22
248	Si-embedded boron-nitride nanotubes as an efficient and metal-free catalyst for NO oxidation. *Superlattices and Microstructures*, **2015**, 81, 7-15	2.8	22
247	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
246	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
245	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	8.5	21
244	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

243	Pnicogen□nicogen interactions in O2XP:PH2Y complexes (X=H, F, CN; Y=H, OH, OCH3, CH3, NH2). *Chemical Physics Letters*, **2015**, 638, 122-127	2.5	20
242	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
241	A comparative study of the CO oxidation reaction over pristine and C-doped boron nitride fullerene. *RSC Advances*, **2016**, 6, 17172-17178	3.7	20
240	Exploring □erogen□ydride□nteractions between ZOF2 (Z = Kr, Xe) and metal hydrides: An ab initio study. *Chemical Physics Letters*, **2016**, 654, 23-28	2.5	20
239	The triel bond: a potential force for tuning anion□nteractions. *Molecular Physics*, **2018**, 116, 388-398	1.7	20
238	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
237	An ab initio study on tunability of □hole interactions in XHS:PH2Y and XH2P:SHY complexes (X = F, Cl, Br; Y = H, OH, OCH3, CH3, C2H5, and NH2). *Journal of Molecular Modeling*, **2015**, 21, 176	2	19
236	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
235	The dual role of halogen, chalcogen, and pnictogen atoms as Lewis acid and base: Triangular XBr:SHX:PH2X complexes (X = F, Cl, Br, CN, NC, OH, NH2, and OCH3). *International Journal of Quantum Chemistry*, **2015**, 115, 1580-1586	2.1	19
234	□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
233	Catalytic dehydrogenation of hydrazine on silicon-carbide nanotubes: A DFT study on the kinetic issue. *Surface Science*, **2015**, 632, 118-125	1.8	18
232	Synthesis, structural characterization and DFT calculations of a new one-dimensional diorganotin(IV) derivative of N-isonicotinyl phosphoramide. *Polyhedron*, **2014**, 71, 8-16	2.7	18
231	Cooperative interaction between □hole and single-electron □hole interactions in O2S□□NCX□□CH3 and O2Se□□NCX□□CH3 complexes (X = F, Cl, Br and I). *Molecular Physics*, **2014**, 112, 2078-2084	1.7	18
230	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	1.9	18
229	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
228	Exploring □hole bonding in XH3Si□□HMY (X=H, F, CN; M=Be, Mg; Y=H, F, CH3) complexes: a "tetrel-hydride" interaction. *Journal of Molecular Modeling*, **2015**, 21, 60	2	17
227	Efficient dehydrogenation of formic acid using Al 12 N 12 nanocage: A DFT study. *Superlattices and Microstructures*, **2014**, 75, 17-26	2.8	17
226	Theoretical study on cooperative effects between X?N and X?Carbene halogen bonds (X = F,Cl,Br and I). *Journal of Molecular Modeling*, **2013**, 19, 4797-804	2	17

225	Cooperative effects between tetrel bond and other σ-hole bond interactions: a comparative investigation. *Molecular Physics*, **2015**, 113, 3703-3711	1.7	17
224	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
223	Computational mechanistic insights into CO oxidation reaction over Fe decorated C24N24 fullerene. *Inorganic Chemistry Communication*, **2019**, 106, 190-196	3.1	16
222	A DFT study on SO3 capture and activation over Si- or Al-doped graphene. *Chemical Physics Letters*, **2016**, 658, 146-151	2.5	16
221	An ab initio study on competition between pnicogen and chalcogen bond interactions in binary XHS:PH2X complexes (X = F, Cl, CCH, COH, CH3, OH, OCH3 and NH2). *Molecular Physics*, **2016**, 114, 1847-1855	1.7	16
220	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	16
219	Substituent effects on cooperativity between lithium bonds. *International Journal of Quantum Chemistry*, **2014**, 114, 295-301	2.1	16
218	A theoretical evidence for cooperativity effects in fluorine-centered halogen bonds: linear (FCN)2F and (FNC)2F clusters. *Structural Chemistry*, **2014**, 25, 403-408	1.8	16
217	Adsorption and decomposition of formaldehyde on the B12N12 nanostructure: a density functional theory study. *Monatshefte Für Chemie*, **2017**, 148, 1727-1731	1.4	16
216	An ab initio study on the concerted interaction between chalcogen and pnicogen bonds. *Journal of Molecular Modeling*, **2014**, 20, 2545	2	16
215	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
214	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
213	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
212	B-doped C3N monolayer: a robust catalyst for oxidation of carbon monoxide. *Theoretical Chemistry Accounts*, **2019**, 138, 1	1.9	15
211	Interplay between hydrogen bond and single-electron tetrel bond: H3C?COX2?HY and H3C?CSX2?HY (X = F, Cl; Y = CN, NC) complexes as a working model. *Computational and Theoretical Chemistry*, **2015**, 1074, 101-106	2	15
210	A computational study on the strength and nature of bifurcated aerogen bonds. *Chemical Physics Letters*, **2018**, 698, 1-6	2.5	15
209	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
208	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

207	Substituent effects on cooperativity of pnicogen bonds. *Journal of Molecular Modeling*, **2014**, 20, 2436	2	15
206	Halogen bonds enhanced by σ-hole and π-hole interactions: a comparative study on cooperativity and competition effects between XN and SN interactions in H3NXCNSF2 and H 3NXCNSO2 complexes (X = F, Cl, Br and I). *Journal of Molecular Modeling*, **2014**, 20, 2291	2	15
205	Competition and interplay between the lithium bonding and hydrogen bonding: RCHHYLiY and RCLiYHY triads as a working model (R=H, CH; Y=CN, NC). *Journal of Molecular Modeling*, **2013**, 19, 5031-5	2	15
204	An ab initio study on anionic aerogen bonds. *Chemical Physics Letters*, **2017**, 667, 337-344	2.5	15
203	An ab initio study on the nature of π-hole interactions in pnicogen-bonded complexes with carbene as an electron donor. *Molecular Physics*, **2016**, 114, 2115-2122	1.7	15
202	A first-principles study on the adsorption behaviour of methanol and ethanol over C59B heterofullerene. *Molecular Physics*, **2017**, 115, 1633-1641	1.7	14
201	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
200	Triphenyltin(IV) adducts of diphosphoryl ligands: structural, electronic and energy aspects from X-ray crystallography and theoretical calculations. *RSC Advances*, **2015**, 5, 17482-17492	3.7	14
199	Cooperative effects in cyclic LiCN and HCN clusters: A comparative study. *Computational and Theoretical Chemistry*, **2013**, 1022, 115-120	2	14
198	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
197	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	4.4	13
196	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
195	Catalytic activity of silicon carbide nanotubes and nanosheets for oxidation of CO: a DFT study. *New Journal of Chemistry*, **2016**, 40, 2775-2784	3.6	12
194	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
193	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, 585-99	4.4	12
192	Theoretical study on cooperative interplay between anion-π and chalcogen-bonding interactions. *Molecular Physics*, **2015**, 113, 1442-1450	1.7	12
191	Exploring lithium bonding interactions between noble-gas hydrides HXeY and LiX molecules (Y=H, CN, NC and X=H, CN, NC, OH, NH2, CH3): A theoretical study. *Computational and Theoretical Chemistry*, **2014**, 1027, 84-90	2	12
190	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

189	Development of TiO2 nanofibers based semiconducting humidity sensor: adsorption kinetics and DFT computations. *Materials Chemistry and Physics*, **2020**, 239, 121981	4.4	12
188	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
187	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
186	Chalcogen bonds tuned by an N□H□□□or C□H□□□nteraction: investigation of substituent, cooperativity and solvent effects. *Molecular Physics*, **2017**, 115, 1713-1723	1.7	11
185	Tuning aerogen bonds via anion-□or lone pair-□nteraction: a comparative ab initio study. *Structural Chemistry*, **2017**, 28, 1255-1264	1.8	11
184	Substituent effects in cooperativity of chalcogen bonds. *Molecular Physics*, **2015**, 113, 3282-3290	1.7	11
183	Intrachain antiferromagnetic exchange in a 1D branched-chain built of two different copper(II) centres interlinked by end-on azido and phenoxo bridges: electron density map, electrochemical and magnetic properties. *RSC Advances*, **2015**, 5, 59926-59934	3.7	11
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