R Chandiramouli

List of Publications by Year in Descending Order

224 papers	4,046 citations	31 h-index	41 g-index
230 ext. papers	4,592 ext. citations	2.9 avg, IF	7.31 L-index

#	Paper	IF	Citations
224	Methylcyclohexane and methyl methacrylate sensing studies using arsenene nanoribbon – A first-principles investigation. *Computational and Theoretical Chemistry*, **2022**, 1209, 113595	2	3
223	DFT study on the adsorption properties of aldrin and dieldrin molecules on blue phosphorene nanotubes. *Physica B: Condensed Matter*, **2022**, 626, 413545	2.8	6
222	Adsorption studies of 2,3-butanedione and acetic acid on phosphorene sheets based on the first-principles study. *Computational and Theoretical Chemistry*, **2022**, 1208, 113548	2	5
221	Recent advances in arsenene nanostructures towards prediction, properties, synthesis and applications. *Surfaces and Interfaces*, **2022**, 28, 101610	4.1	5
220	Adsorption studies of SF6 and decomposed constituents on 4B arsenene nanotubes – A first-principles study. *Computational and Theoretical Chemistry*, **2022**, 1211, 113663	2	1
219	Chemisorption of atrazine and diuron molecules on arsenene nanosheet - a first-principles study. *Chemical Physics Letters*, **2022**, 794, 139484	2.5	3
218	Carbonyl sulfide and dimethyl sulfide adsorption studies on novel square-octagon antimonene sheets – A first-principles study. *Chemical Physics*, **2022**, 558, 111504	2.3	0
217	Sorption studies of dimethyl sulfoxide and tetrahydrofuran on gamma arsenene nanotubes – A first-principles study. *Applied Surface Science*, **2022**, 592, 153210	6.7	1
216	Tetrahydrofuran and 2-Methyltetrahydrofuran adsorption studies on violet phosphorene nanosheets based on first-principles studies. *Journal of Molecular Liquids*, **2022**, 119062	6	3
215	SF6 and SOF2 interaction studies on novel Tricycle Red Phosphorene sheets based on first-principles studies. *Chemical Physics Letters*, **2022**, 139674	2.5	1
214	Physisorption of trichloroethylene and tetrachloroethylene on novel zeta arsenene nanotubes – A first-principles study. *Journal of Molecular Graphics and Modelling*, **2022**, 108233	2.8	0
213	Electronic and band structure studies on In and N doped Ga2O3 nanostructures from first-principles calculations. *Materials Today: Proceedings*, **2021**, 47, 6418-6428	1.4	
212	Structural and electronic properties of InGaAs, InGaP and InGaSb nanostructures – A density functional theory approach. *Materials Today: Proceedings*, **2021**, 47, 6489-6498	1.4	
211	Molecular interaction studies of styrene on single and double-walled square-octagon phosphorene nanotubes – First-principles investigation. *Chemical Physics Letters*, **2021**, 785, 139149	2.5	14
210	Interaction studies of liver cancer biomarkers on black phosphorene sheets – A DFT outlook. *FlatChem*, **2021**, 30, 100293	5.1	6
209	Molecular adsorption of o-ethyltoluene and phenyl propane on square-octagon phosphorene nanosheet – A first-principles calculation. *Journal of Molecular Liquids*, **2021**, 326, 115320	6	25
208	Interaction studies of nitrotoluene and toluidine molecules on novel square-octagon arsenene nanotubes based on DFT method. *Journal of Molecular Liquids*, **2021**, 325, 115260	6	15

207	Molecular interaction of oxytetracycline and sulfapyridine on blue phosphorene nanotubes: A first-principles insight. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2021**, 394, 127198	2.3	12
206	Kagome phosphorene molecular device for sensing chloropicrin and phosgene – A first-principles study. *Chemical Physics Letters*, **2021**, 771, 138472	2.5	28
205	Chlorobenzene and 1, 4-dichlorobenzene adsorption studies on Arsenene nanosheet – a first-principles analysis. *Molecular Physics*, **2021**, 119, e1936248	1.7	8
204	Interaction studies of glycine, acetate and methylamine on Tellurene nanoribbon - A first-principles analysis. *Journal of Molecular Graphics and Modelling*, **2021**, 105, 107895	2.8	15
203	Interaction studies of diclofenac and ibuprofen molecules on armchair bismuthene nanotubes: A first-principles study. *Chemical Physics*, **2021**, 546, 111169	2.3	14
202	Sorption studies and removal of chlortetracycline and oxytetracycline using theta phosphorene nanoribbon – A DFT outlook. *Journal of Molecular Liquids*, **2021**, 117070	6	9
201	First-principles studies on sensing properties of delta arsenene nanoribbons towards hexane and heptane molecules. *Computational and Theoretical Chemistry*, **2021**, 1201, 113256	2	13
200	Molecular interaction studies of cumene and toluene on arsenene nanosheet – a first-principles outlook. *Molecular Physics*, **2021**, 119, e1800853	1.7	18
199	Chemisorption of Heptachlor and Mirex molecules on beta arsenene nanotubes – A first-principles analysis. *Applied Surface Science*, **2021**, 537, 147835	6.7	24
198	Square-octagon arsenene nanosheet as chemical nanosensor for M-xylene and toluene – A DFT outlook. *Computational and Theoretical Chemistry*, **2021**, 1196, 113088	2	17
197	First-principles research on adsorption properties of o-xylene and styrene on 58 phosphorene sheets. *Chemical Physics Letters*, **2021**, 765, 138244	2.5	27
196	Adsorption studies of nucleobases on arsenene nanosheet based on first-principles research. *Journal of Molecular Graphics and Modelling*, **2021**, 103, 107827	2.8	15
195	Chemiresistive Tellurene nanosheets for detecting 2-Butanone and 2-Pentanone - a first-principles study. *Materials Today Communications*, **2021**, 26, 101758	2.5	5
194	Alcohol molecular interaction studies on stair phosphorene nanosheets: a first-principles approach. *Structural Chemistry*, **2021**, 32, 27-36	1.8	15
193	Chemosensing nature of black phosphorene nanotube towards C14H9Cl5 and C10H5Cl7 molecules – A first-principles insight. *Computational and Theoretical Chemistry*, **2021**, 1196, 113109	2	11
192	Red tricycle phosphorene nanoribbon as a removing medium of sulfadiazine and sulfamethoxazole molecules based on first-principles studies. *Journal of Molecular Liquids*, **2021**, 336, 116294	6	20
191	Chemisorption of sulfaguanidine and sulfanilamide drugs on bismuthene nanosheet based on first-principles studies. *Applied Surface Science*, **2021**, 561, 149990	6.7	9
190	Adsorption behaviour of trichloropropane and tetrachloroethylene on phosphorene sheets: A first-principles insight. *Computational and Theoretical Chemistry*, **2021**, 1203, 113347	2	15

189	Interaction studies of dichlobenil and isoproturon on square-octagon phosphorene nanotube based on DFT frame work. *Chemical Physics Letters*, **2021**, 778, 138773	2.5	17
188	Zipper phosphorene as sensing element towards formaldehyde and acetaldehyde - A first-principles insight. *Journal of Molecular Graphics and Modelling*, **2021**, 107, 107971	2.8	14
187	Interaction of propionate and ethylamine on kagome phosphorene nanoribbons – A DFT study. *Chemical Physics*, **2021**, 549, 111276	2.3	11
186	Interaction studies of benzene and phenol on novel 4–8 arsenene nanotubes – A DFT insight. *Computational and Theoretical Chemistry*, **2021**, 1204, 113381	2	8
185	Interaction studies of tuberculosis biomarker vapours on novel beta arsenene sheets – A DFT insight. *Computational and Theoretical Chemistry*, **2021**, 1205, 113426	2	10
184	Sorption studies of sulfadimethoxine and tetracycline molecules on –antimonene nanotube - A first-principles insight. *Journal of Molecular Graphics and Modelling*, **2021**, 108, 107988	2.8	8
183	Adsorption behaviour of sulfisoxazole molecules on tricycle arsenene nanoribbon - a first-principles study. *Journal of Molecular Liquids*, **2021**, 343, 117635	6	14
182	Twisted bilayer arsenene sheets as a chemical sensor for toluene and M-xylene vapours - A DFT investigation. *Journal of Molecular Graphics and Modelling*, **2021**, 109, 108034	2.8	9
181	Molecular Modeling and Simulation of glycine functionalized B12N12 and B16N16 nanoclusters as potential inhibitors of proinflammatory cytokines. *Journal of Molecular Liquids*, **2021**, 343, 117494	6	7
180	Novel –arsenene nanosheets for sensing toxic malathion and parathion – A first-principles approach. *Computational and Theoretical Chemistry*, **2020**, 1190, 112995	2	13
179	Interaction studies of volatiles from jackfruit on –phosphorene nanosheets– DFT outlook. *Structural Chemistry*, **2020**, 31, 1851-1860	1.8	15
178	Novel gamma arsenene nanosheets as sensing medium for vomiting agents: A first-principles research. *Computational and Theoretical Chemistry*, **2020**, 1185, 112876	2	19
177	Interaction studies of aniline on pristine and Al-doped –Arsenene nanosheets – A first-principles insight. *Chemical Physics Letters*, **2020**, 752, 137588	2.5	32
176	Physisorption of propane and butane vapors on novel Kagome antimonene sheets – A first-principles perception. *Chemical Physics Letters*, **2020**, 754, 137693	2.5	28
175	Surface assimilation studies of ethyl methyl sulfide on gamma phosphorene sheets – a DFT outlook. *Molecular Physics*, **2020**, 118, e1774089	1.7	12
174	Investigation on adsorption properties of HCN and ClCN blood agents on –phosphorene nanosheets – A first–principles insight. *Chemical Physics*, **2020**, 538, 110896	2.3	28
173	Interaction study of amino acid on novel Kagome phosphorene nanotube – A DFT outlook. *Computational and Theoretical Chemistry*, **2020**, 1186, 112903	2	21
172	Methyl and Ethyl mercaptan molecular adsorption studies on novel Kagome arsenene nanosheets - A DFT outlook. *Physica B: Condensed Matter*, **2020**, 586, 412135	2.8	28

171	Novel □phosphorene nanosheet device for the detection of tear gas molecules □A first-principles research. *Chemical Physics Letters*, **2020**, 747, 137353	2.5	35
170	Computational Studies on the Interaction of Formaldehyde Vapor with □Phosphorene Nanosheet: A DFT Insight. *ChemistrySelect*, **2020**, 5, 3398-3404	1.8	19
169	Surface adsorption studies of benzyl bromide and bromobenzyl cyanide vapours on black phosphorene nanosheets □a first-principles perception. *Molecular Physics*, **2020**, 118, e1737744	1.7	14
168	Halomethane Adsorption Studies on Silicane Sheets: A First-Principles Perception. *Journal of Inorganic and Organometallic Polymers and Materials*, **2020**, 30, 3263-3275	3.2	13
167	DFT Outlook on Surface Adsorption Properties of Nitrobenzene on Novel Red Tricycle Arsenene Nanoring. *Journal of Inorganic and Organometallic Polymers and Materials*, **2020**, 30, 4329-4341	3.2	11
166	First-principles perspectives on detection properties of sulphur mustard gas using novel electroresistive ?-Arsenene nanosheet device. *Molecular Physics*, **2020**, 118, e1725671	1.7	9
165	Graphdiyne nanosheets as a sensing medium for formaldehyde and formic acid □A first-principles outlook. *Computational and Theoretical Chemistry*, **2020**, 1176, 112751	2	34
164	Interaction studies of kidney biomarker volatiles on black phosphorene nanoring: A first-principles investigation. *Journal of Molecular Graphics and Modelling*, **2020**, 97, 107566	2.8	32
163	Adamsite and chloropicrin molecular adsorption studies on novel green phosphorene nanotube □ First-principles investigation. *Chemical Physics*, **2020**, 535, 110782	2.3	24
162	Arsenic pentafluoride surface adsorption studies on Kagome-phosphorene □a DFT outlook. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2020**, 384, 126552	2.3	16
161	Toxicants in cigarette smoke adsorbed on red phosphorene nanosheet: A first-principles insight. *Chemical Physics*, **2020**, 530, 110604	2.3	18
160	Expedition on surface adsorption of N-nitrosodiethylamine from rubber fumes on blue phosphorene sheets □a first-principles insight. *Molecular Physics*, **2020**, 118, e1699184	1.7	10
159	N-nitrosodimethylamine interaction studies on gamma phosphorene sheets emitted from rubber fumes □A first-principles study. *Physica B: Condensed Matter*, **2020**, 577, 411808	2.8	14
158	Explosive vapor detection using novel graphdiyne nanoribbons□ first-principles investigation. *Structural Chemistry*, **2020**, 31, 709-717	1.8	15
157	Exploring adsorption behavior of ethylene dichloride and dibromide vapors on blue phosphorene nanosheets: A first-principles acumens. *Journal of Molecular Graphics and Modelling*, **2020**, 95, 107505	2.8	19
156	Sensing studies of DDT and Toxaphene molecules using chemi-resistive □antimonene nanotubes based on first-principles insights. *Chemical Physics Letters*, **2020**, 757, 137895	2.5	17
155	Dimethyl and ethyl methyl ether adsorption studies on □antimonene nanosheets □a first-principles study. *Molecular Simulation*, **2020**, 46, 1354-1361	2	12
154	Molecular adsorption studies of diethyl sulfide and ethyl methyl sulfide vapors on □phosphorene nanoribbon □A first-principles insight. *Applied Surface Science*, **2020**, 534, 147597	6.7	22

153	Investigation on adsorption features of nitroglycerin on novel red tricycle arsenene nanosheet - A first-principles study. *Journal of Molecular Graphics and Modelling*, **2020**, 100, 107653	2.8	10
152	Molecular adsorption studies of benzidine on novel Kagome antimonene nanosheets - Insights based on first-principles DFT calculations. *Journal of Molecular Liquids*, **2020**, 318, 113972	6	15
151	Benzyl alcohol and 2-methyldecalin vapor adsorption studies on bismuthene sheets A DFT outlook. *Chemical Physics Letters*, **2020**, 755, 137819	2.5	19
150	Interaction properties of phenol and styrene from plastic fumes on Arsenene sheets: A first-principles study. *Physica B: Condensed Matter*, **2020**, 597, 412405	2.8	13
149	First-principles insight on interaction behavior of diethylbenzene and ethyltoluene on arsenene nanoring. *Materials Today Communications*, **2020**, 25, 101476	2.5	2
148	Novel green phosphorene sheets to detect tear gas molecules - A DFT insight. *Journal of Molecular Graphics and Modelling*, **2020**, 100, 107706	2.8	21
147	Boron trifluoride interaction studies on graphdiyne nanotubes A first-principles insight. *Chemical Physics Letters*, **2020**, 738, 136841	2.5	32
146	Benzyl Chloride and Chlorobenzene Adsorption Studies on Bismuthene Nanosheet: A DFT Study. *Journal of Inorganic and Organometallic Polymers and Materials*, **2020**, 30, 1888-1897	3.2	12
145	Investigation on graphdiyne nanosheet in adsorption of sorafenib and regorafenib drugs: A DFT approach. *Journal of Molecular Liquids*, **2019**, 277, 776-785	6	56
144	Probing cyanogen chloride gas molecules using blue phosphorene nanosheets based on adsorption properties: A first-principles study. *Computational and Theoretical Chemistry*, **2019**, 1150, 63-70	2	31
143	Adsorption studies of dimethyl and methyl-ethyl ester molecules on silicene nanoring: Application of DFT study. *Phosphorus, Sulfur and Silicon and the Related Elements*, **2019**, 194, 25-32	1	10
142	First-principles studies on mechanical properties and band structures of TMO2 (TM = Zr or Hf) nanostructures under high pressure. *Physica B: Condensed Matter*, **2019**, 559, 1-7	2.8	11
141	First-principles investigation on detection of phosgene gas molecules using phosphorene nanosheet device. *Chemical Physics Letters*, **2019**, 717, 99-106	2.5	44
140	Silicene nanosheet device with nanopore to identify the nucleobases A first-principles perspective. *Chemical Physics Letters*, **2019**, 730, 70-75	2.5	21
139	Graphyne nanotube as nanofilter for cigarette smoke based on chemisorption properties A first-principles study. *Diamond and Related Materials*, **2019**, 97, 107436	3.5	7
138	DFT Study on the Interaction Properties of V-Series Nerve Agent Molecules on Novel Bismuthene Nanotubes. *Journal of Inorganic and Organometallic Polymers and Materials*, **2019**, 29, 2226-2236	3.2	18
137	First-principles analysis of the detection of amine vapors using an antimonene electroresistive molecular device. *Journal of Computational Electronics*, **2019**, 18, 779-790	1.8	14
136	Perceptions on the adsorption of COPD biomarker vapors on violet phosphorene nanosheet - A first-principles study. *Journal of Molecular Graphics and Modelling*, **2019**, 91, 22-29	2.8	22

135	Adsorption Ability of Germanane Nanosheets Towards Nitrogen and Sulfur Mustard Gas Molecules: A First-Principles Study. *Journal of Inorganic and Organometallic Polymers and Materials*, **2019**, 29, 2035-2043	3.2	8
134	Investigation on bare and hydrogenated Sb-nanosheets as an electrode material for Na-ion battery - A DFT study. *Physica B: Condensed Matter*, **2019**, 562, 75-81	2.8	26
133	Diethanolamine and quaternium-15 interaction studies on antimonene nanosheet based on first-principles studies. *Computational and Theoretical Chemistry*, **2019**, 1157, 19-27	2	24
132	Exploring adsorption mechanism of hydrogen cyanide and cyanogen chloride molecules on arsenene nanoribbon from first-principles. *Journal of Molecular Graphics and Modelling*, **2019**, 89, 13-21	2.8	30
131	Adsorption insights of amine vapors on black phosphorene nanotubes□ first-principles study. *Materials Research Express*, **2019**, 6, 105518	1.7	9
130	Nitrogen mustard gas molecules and □arsenene nanosheet interaction studies - A DFT insight. *Journal of Molecular Graphics and Modelling*, **2019**, 92, 65-73	2.8	20
129	Adsorption behavior of cytosine and guanine nucleobases on graphyne nanosheets: A DFT study. *Computational and Theoretical Chemistry*, **2019**, 1163, 112514	2	21
128	Acrylonitrile vapor adsorption studies on armchair arsenene nanoribbon based on DFT study. *Applied Surface Science*, **2019**, 494, 1148-1155	6.7	18
127	Interaction properties of explosive vapors on □graphyne nanosheet □a DFT outlook. *Fullerenes Nanotubes and Carbon Nanostructures*, **2019**, 27, 770-778	1.8	10
126	Flutamide drug interaction studies on graphdiyne nanotube □A first-principles study. *Computational and Theoretical Chemistry*, **2019**, 1167, 112590	2	18
125	Interaction properties of benzyl chloride and chlorobenzene on violet phosphorene sheets □A first-principles perception. *Computational and Theoretical Chemistry*, **2019**, 1165, 112563	2	18
124	Electronic properties of novel bismuthene nanosheets with adsorption studies of G-series nerve agent molecules □a DFT outlook. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2019**, 383, 125975	2.3	17
123	Mechanical properties and band structure of CdSe and CdTe nanostructures at high pressure - a first-principles study. *Processing and Application of Ceramics*, **2019**, 13, 124-131	1.4	10
122	Blue phosphorene nanoribbon for detection of chloroform vapours □a first-principles study. *International Journal of Environmental Analytical Chemistry*, **2019**, 1-13	1.8	8
121	Interaction Studies of Methanol and Ethanol Vapors on Green Phosphorene Sheets: A First-Principles Study. *ChemistrySelect*, **2019**, 4, 14237-14243	1.8	13
120	Detection of trace level of hazardous phosgene gas on antimonene nanotube based on first-principles method. *Journal of Molecular Graphics and Modelling*, **2019**, 88, 32-40	2.8	32
119	Investigation on probing explosive nitroaromatic compound vapors using graphyne nanosheet: a first-principle study. *Structural Chemistry*, **2019**, 30, 657-667	1.8	17
118	Germanene nanosheets as a novel anode material for sodium-ion batteries□ first-principles investigation. *Materials Research Express*, **2019**, 6, 035504	1.7	20

117	A study on quercetin and 5-fluorouracil drug interaction on graphyne nanosheets and solvent effects – A first-principles study. *Journal of Molecular Liquids*, **2019**, 275, 713-722	6	39
116	Germanane nanosheet as a novel biosensor for liver cirrhosis based on adsorption of biomarker volatiles – A DFT study. *Applied Surface Science*, **2019**, 475, 990-998	6.7	41
115	Interaction Behavior of Cyanogen Fluoride and Chloride Gas Molecules on Red Phosphorene Nanosheet: A DFT Study. *Journal of Inorganic and Organometallic Polymers and Materials*, **2019**, 29, 954-963	3.2	27
114	Mechanical and electronic properties under high pressure on ternary AlGaN and InGaN compounds– first-principles perspective. *Materials Research Express*, **2019**, 6, 015052	1.7	12
113	Arsenene nanoribbons for sensing NH3 and PH3 gas molecules – A first-principles perspective. *Applied Surface Science*, **2019**, 469, 173-180	6.7	63
112	Germanene nanotube electroresistive molecular device for detection of NO2 and SO2 gas molecules: a first-principles investigation. *Journal of Computational Electronics*, **2019**, 18, 308-318	1.8	19
111	MoSe nanosheets for detection of methanol and ethanol vapors: A DFT study. *Journal of Molecular Graphics and Modelling*, **2018**, 81, 97-105	2.8	31
110	DFT investigation on the adsorption behavior of dimethyl and trimethyl amine molecules on borophene nanotube. *Chemical Physics Letters*, **2018**, 701, 34-42	2.5	26
109	Investigation on adsorption properties of CO and NO gas molecules on aluminene nanosheet: A density functional application. *Materials Science and Engineering B: Solid-State Materials for Advanced Technology*, **2018**, 229, 193-200	3.1	36
108	Adsorption behavior of NH3 and NO2 molecules on stanene and stanane nanosheets – A density functional theory study. *Chemical Physics Letters*, **2018**, 695, 162-169	2.5	40
107	First-Principles Insights on Acetone Vapor Manganese Ferrite Solid Surface Interactions. *Journal of Inorganic and Organometallic Polymers and Materials*, **2018**, 28, 121-129	3.2	6
106	Alcohol molecules adsorption on graphane nanosheets – A first-principles investigation. *Applied Surface Science*, **2018**, 441, 734-743	6.7	31
105	Density functional studies on the binding of methanol and ethanol molecules to graphyne nanosheet. *Computational and Theoretical Chemistry*, **2018**, 1125, 86-94	2	46
104	Interaction of volatile organic compounds (VOCs) emitted from banana on stanene nanosheet– first-principles studies. *Structural Chemistry*, **2018**, 29, 1321-1332	1.8	15
103	Adsorption studies of volatile organic compounds on germanene nanotube emitted from banana fruit for quality assessment - A density functional application. *Journal of Molecular Graphics and Modelling*, **2018**, 82, 129-136	2.8	16
102	DFT Application on the Interaction Properties of Ethanol Vapors with MnFe2O4 Nanostructures. *Journal of Inorganic and Organometallic Polymers and Materials*, **2018**, 28, 1753-1763	3.2	7
101	A novel approach for detection of NO 2 and SO 2 gas molecules using graphane nanosheet and nanotubes - A density functional application. *Diamond and Related Materials*, **2018**, 85, 53-62	3.5	24
100	Detection of nucleobases using 2D germanane nanosheet: A first-principles study. *Computational and Theoretical Chemistry*, **2018**, 1130, 68-76	2	26

99	First-principles studies on electronic properties of Oligo-p-phenylene molecular device. *Solid State Communications*, **2018**, 269, 50-57	1.6	11
98	First-principles investigation on transport properties of (hbox {Zn}_{2}hbox {SnO}_{4}) molecular device and response toward (hbox {NO}_{2}) gas molecules. *Journal of Computational Electronics*, **2018**, 17, 1-8	1.8	14
97	Novel method to detect the lung cancer biomarker volatiles using hydrogen vacant silicane nanosheets: A DFT investigation. *Computational and Theoretical Chemistry*, **2018**, 1138, 107-116	2	20
96	First-principles insights on the electronic and field emission properties of Ga and Al doped germanium nanocones. *Journal of Electron Spectroscopy and Related Phenomena*, **2018**, 227, 15-22	1.7	15
95	Nucleobases adsorption studies on silicane layer: A first-principles investigation. *Journal of Molecular Graphics and Modelling*, **2018**, 85, 48-55	2.8	14
94	Antimonene nanosheet device for detection of explosive vapors A first-principles inspection. *Chemical Physics Letters*, **2018**, 708, 130-137	2.5	37
93	Density functional study on the binding properties of nucleobases to stanane nanosheet. *Applied Surface Science*, **2018**, 462, 831-839	6.7	22
92	Arsenene Nanotube as a Chemical Sensor to Detect the Presence of Explosive Vapors: A First-Principles Insight. *Journal of Inorganic and Organometallic Polymers and Materials*, **2018**, 28, 2844-2853	3.2	27
91	Doped aluminum nanocones as an efficient electron field emitter: A first-principles investigation. *Inorganic Chemistry Communication*, **2018**, 96, 5-12	3.1	14
90	First-principles investigation on switching properties of spiropyran and merocyanine grafted graphyne nanotube device. *Chemical Physics Letters*, **2018**, 691, 37-43	2.5	30
89	Adsorption of ammonia molecules and humidity on germanane nanosheet-A density functional study. *Journal of Molecular Graphics and Modelling*, **2018**, 79, 149-156	2.8	25
88	High-pressure studies on electronic and mechanical properties of FeBO3 (B = Ti, Mn, Cr) ceramics a first-principles study. *Phase Transitions*, **2018**, 91, 382-397	1.3	12
87	Adsorption studies of trimethyl amine and n-butyl amine vapors on stanene nanotube molecular device A first-principles study. *Chemical Physics*, **2018**, 501, 78-85	2.3	26
86	First-principles insights on detection of dimethyl amine and trimethyl amine vapors using graphdiyne nanosheets. *Computational and Theoretical Chemistry*, **2018**, 1123, 119-127	2	42
85	Interaction Studies of Ammonia Gas Molecules on Borophene Nanosheet and Nanotubes: A Density Functional Study. *Journal of Inorganic and Organometallic Polymers and Materials*, **2018**, 28, 920-931	3.2	12
84	First-principles investigation on structural and electronic properties of antimonene nanoribbons and nanotubes. *Physica E: Low-Dimensional Systems and Nanostructures*, **2018**, 97, 98-104	3	39
83	Investigation of NH3 adsorption behavior on graphdiyne nanosheet and nanotubes: A first-principles study. *Journal of Molecular Liquids*, **2018**, 249, 24-32	6	51
82	Novel bismuthene nanotubes to detect NH3, NO2 and PH3 gas molecules A first-principles insight. *Chemical Physics Letters*, **2018**, 712, 102-111	2.5	34

81	Interaction of Imuran, Pentasa and Hyoscyamine drugs and solvent effects on graphdiyne nanotube as a drug delivery system - A DFT study. *Journal of Molecular Liquids*, **2018**, 265, 199-207	6	42
80	Borophene nanosheet molecular device for detection of ethanol – A first-principles study. *Computational and Theoretical Chemistry*, **2017**, 1105, 52-60	2	54
79	Sensing properties of monolayer borophane nanosheet towards alcohol vapors: A first-principles study. *Journal of Molecular Graphics and Modelling*, **2017**, 73, 208-216	2.8	35
78	First-Principles Insights of CO Adsorption Characteristics on Ge and In Substituted Silicene Nanosheet. *Silicon*, **2017**, 9, 327-337	2.4	15
77	Investigation of electronic properties and spin-orbit coupling effects on passivated stanene nanosheet: A first-principles study. *Superlattices and Microstructures*, **2017**, 107, 118-126	2.8	18
76	Interaction of alcohols on monolayer stanane nanosheet: A first-principles investigation. *Applied Surface Science*, **2017**, 419, 9-15	6.7	23
75	Borospherene nanostructure as CO and NO sensor – A first-principles study. *Vacuum*, **2017**, 142, 13-20	3.7	38
74	Adsorption of NO molecules on armchair phosphorene nanosheet for nano sensor applications - A first-principles study. *Journal of Molecular Graphics and Modelling*, **2017**, 75, 365-374	2.8	43
73	Adsorption studies of ethanol and butanol on Co3O4 nanostructures – A DFT study. *Chemical Physics*, **2017**, 491, 61-68	2.3	19
72	Study of Alcohol and Aldehydes Interaction on the Surface of Silicane Nanosheet: Application of Density Functional Theory. *Journal of Inorganic and Organometallic Polymers and Materials*, **2017**, 27, 1307-1316	3.2	14
71	Adsorption studies of alcohol molecules on monolayer MoS2 nanosheet–A first-principles insights. *Applied Surface Science*, **2017**, 413, 109-117	6.7	54
70	CO and NO monitoring using pristine germanene nanosheets: DFT study. *Journal of Molecular Liquids*, **2017**, 234, 355-363	6	27
69	Transport studies of (hbox {CeO}_{2}) molecular device and adsorption behavior of CO on (hbox {CeO}_{2}) device: a first-principles investigation. *Journal of Computational Electronics*, **2017**, 16, 316-324	1.8	10
68	Switching properties of quinquephenylene molecular device – A first-principles approach. *Chemical Physics Letters*, **2017**, 675, 131-136	2.5	16
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