R Chandiramouli

List of Publications by Citations

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	Review of CdO thin films. *Solid State Sciences*, **2013**, 16, 102-110	3.4	110
223	NO adsorption studies on silicene nanosheet: DFT investigation. *Applied Surface Science*, **2015**, 351, 662-672	6.7	70
222	Arsenene nanoribbons for sensing NH3 and PH3 gas molecules A first-principles perspective. *Applied Surface Science*, **2019**, 469, 173-180	6.7	63
221	Investigation on graphdiyne nanosheet in adsorption of sorafenib and regorafenib drugs: A DFT approach. *Journal of Molecular Liquids*, **2019**, 277, 776-785	6	56
220	Borophene nanosheet molecular device for detection of ethanol A first-principles study. *Computational and Theoretical Chemistry*, **2017**, 1105, 52-60	2	54
219	Adsorption studies of alcohol molecules on monolayer MoS2 nanosheetA first-principles insights. *Applied Surface Science*, **2017**, 413, 109-117	6.7	54
218	Investigation of NH3 adsorption behavior on graphdiyne nanosheet and nanotubes: A first-principles study. *Journal of Molecular Liquids*, **2018**, 249, 24-32	6	51
217	Operating temperature dependent ethanol and formaldehyde detection of spray deposited mixed CdO and MnO2 thin films. *RSC Advances*, **2015**, 5, 43930-43940	3.7	49
216	Density functional studies on the binding of methanol and ethanol molecules to graphyne nanosheet. *Computational and Theoretical Chemistry*, **2018**, 1125, 86-94	2	46
215	NO2 adsorption behaviour on germanene nanosheet A first-principles investigation. *Superlattices and Microstructures*, **2017**, 101, 160-171	2.8	44
214	First-principles investigation on detection of phosgene gas molecules using phosphorene nanosheet device. *Chemical Physics Letters*, **2019**, 717, 99-106	2.5	44
213	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
212	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
211	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
210	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
209	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
208	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

207	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
206	Borospherene nanostructure as CO and NO sensor – A first-principles study. *Vacuum*, **2017**, 142, 13-20	3.7	38
205	Antimonene nanosheet device for detection of explosive vapors – A first-principles inspection. *Chemical Physics Letters*, **2018**, 708, 130-137	2.5	37
204	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
203	Adsorption studies of NH3 molecules on functionalized germanene nanosheet – A DFT study. *Chemical Physics Letters*, **2016**, 665, 22-30	2.5	36
202	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
201	Novel –phosphorene nanosheet device for the detection of tear gas molecules – A first-principles research. *Chemical Physics Letters*, **2020**, 747, 137353	2.5	35
200	Graphdiyne nanosheets as a sensing medium for formaldehyde and formic acid – A first-principles outlook. *Computational and Theoretical Chemistry*, **2020**, 1176, 112751	2	34
199	TeO2 nanostructures as a NO2 sensor: DFT investigation. *Computational and Theoretical Chemistry*, **2014**, 1049, 20-27	2	34
198	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
197	Interaction studies of aniline on pristine and Al-doped –Arsenene nanosheets – A first-principles insight. *Chemical Physics Letters*, **2020**, 752, 137588	2.5	32
196	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
195	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
194	Boron trifluoride interaction studies on graphdiyne nanotubes – A first-principles insight. *Chemical Physics Letters*, **2020**, 738, 136841	2.5	32
193	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
192	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
191	Alcohol molecules adsorption on graphane nanosheets – A first-principles investigation. *Applied Surface Science*, **2018**, 441, 734-743	6.7	31
190	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

189	First-principles investigation on switching properties of spiropyran and merocyanine grafted graphyne nanotube device. *Chemical Physics Letters*, **2018**, 691, 37-43	2.5	30
188	DFT investigation on CO sensing characteristics of hexagonal and orthorhombic WO3 nanostructures. *Superlattices and Microstructures*, **2015**, 78, 22-39	2.8	29
187	Quantum chemical studies on CdO nanoclusters stability. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 102, 242-9	4.4	29
186	First-Principles Investigation on Interaction of NH3 Gas on a Silicene Nanosheet Molecular Device. *IEEE Nanotechnology Magazine*, **2017**, 16, 445-452	2.6	28
185	Physisorption of propane and butane vapors on novel Kagome antimonene sheets □A first-principles perception. *Chemical Physics Letters*, **2020**, 754, 137693	2.5	28
184	Investigation on adsorption properties of HCN and ClCN blood agents on □hosphorene nanosheets □A first□principles insight. *Chemical Physics*, **2020**, 538, 110896	2.3	28
183	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
182	Kagome phosphorene molecular device for sensing chloropicrin and phosgene □A first-principles study. *Chemical Physics Letters*, **2021**, 771, 138472	2.5	28
181	CO and NO monitoring using pristine germanene nanosheets: DFT study. *Journal of Molecular Liquids*, **2017**, 234, 355-363	6	27
180	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
179	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
178	First-principles research on adsorption properties of o-xylene and styrene on 5□ phosphorene sheets. *Chemical Physics Letters*, **2021**, 765, 138244	2.5	27
177	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
176	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
175	Detection of nucleobases using 2D germanane nanosheet: A first-principles study. *Computational and Theoretical Chemistry*, **2018**, 1130, 68-76	2	26
174	NiO nanocone as a CO sensor: DFT investigation. *Structural Chemistry*, **2014**, 25, 1765-1771	1.8	26
173	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
172	H2S and NH3 adsorption characteristics on CoO nanowire molecular device □A first-principles study. *Chemical Physics Letters*, **2015**, 636, 51-57	2.5	25

171	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
170	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
169	Diethanolamine and quaternium-15 interaction studies on antimonene nanosheet based on first-principles studies. *Computational and Theoretical Chemistry*, **2019**, 1157, 19-27	2	24
168	Adamsite and chloropicrin molecular adsorption studies on novel green phosphorene nanotube □ First-principles investigation. *Chemical Physics*, **2020**, 535, 110782	2.3	24
167	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
166	Chemisorption of Heptachlor and Mirex molecules on beta arsenene nanotubes □A first-principles analysis. *Applied Surface Science*, **2021**, 537, 147835	6.7	24
165	Interaction of alcohols on monolayer stanane nanosheet: A first-principles investigation. *Applied Surface Science*, **2017**, 419, 9-15	6.7	23
164	DFT Studies on Interaction of H2S Gas with □Fe2O3 Nanostructures. *Journal of Inorganic and Organometallic Polymers and Materials*, **2016**, 26, 394-404	3.2	23
163	Structural and electronic properties of germanane nanosheet upon molecular adsorption of alcohol and aldehyde molecules: DFT comparative analysis. *Journal of Molecular Liquids*, **2017**, 242, 571-579	6	23
162	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
161	Density functional study on the binding properties of nucleobases to stanane nanosheet. *Applied Surface Science*, **2018**, 462, 831-839	6.7	22
160	Investigation on band structure and electronic transport properties of indium nitride nanoribbon □ A first-principles study. *Superlattices and Microstructures*, **2014**, 65, 22-34	2.8	22
159	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
158	Silicene nanosheet device with nanopore to identify the nucleobases □A first-principles perspective. *Chemical Physics Letters*, **2019**, 730, 70-75	2.5	21
157	Interaction study of amino acid on novel Kagome phosphorene nanotube □A DFT outlook. *Computational and Theoretical Chemistry*, **2020**, 1186, 112903	2	21
156	Adsorption behavior of cytosine and guanine nucleobases on graphyne nanosheets: A DFT study. *Computational and Theoretical Chemistry*, **2019**, 1163, 112514	2	21
155	Novel green phosphorene sheets to detect tear gas molecules - A DFT insight. *Journal of Molecular Graphics and Modelling*, **2020**, 100, 107706	2.8	21
154	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

153	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
152	Investigation on electronic properties of functionalized arsenene nanoribbon and nanotubes: A first-principles study. *Chemical Physics*, **2017**, 495, 35-41	2.3	20
151	A DFT study on adsorption behaviour of CO on Co3O4 nanostructures. *Applied Surface Science*, **2016**, 385, 113-121	6.7	20
150	Germanene nanosheets as a novel anode material for sodium-ion batteries first-principles investigation. *Materials Research Express*, **2019**, 6, 035504	1.7	20
149	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
148	Adsorption studies of ethanol and butanol on Co3O4 nanostructures A DFT study. *Chemical Physics*, **2017**, 491, 61-68	2.3	19
147	Novel gamma arsenene nanosheets as sensing medium for vomiting agents: A first-principles research. *Computational and Theoretical Chemistry*, **2020**, 1185, 112876	2	19
146	Computational Studies on the Interaction of Formaldehyde Vapor with Phosphorene Nanosheet: A DFT Insight. *ChemistrySelect*, **2020**, 5, 3398-3404	1.8	19
145	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
144	Benzyl alcohol and 2-methyldecalin vapor adsorption studies on bismuthene sheets A DFT outlook. *Chemical Physics Letters*, **2020**, 755, 137819	2.5	19
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142	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
141	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
140	Acrylonitrile vapor adsorption studies on armchair arsenene nanoribbon based on DFT study. *Applied Surface Science*, **2019**, 494, 1148-1155	6.7	18
139	Flutamide drug interaction studies on graphdiyne nanotube A first-principles study. *Computational and Theoretical Chemistry*, **2019**, 1167, 112590	2	18
138	Interaction properties of benzyl chloride and chlorobenzene on violet phosphorene sheets A first-principles perception. *Computational and Theoretical Chemistry*, **2019**, 1165, 112563	2	18
137	First-principles investigation on transport properties of NiO monowire-based molecular device. *Molecular Physics*, **2014**, 112, 1954-1962	1.7	18
136	DFT Investigation of Formaldehyde Adsorption Characteristics on MgO Nanotube. *Journal of Inorganic and Organometallic Polymers and Materials*, **2014**, 24, 1038-1047	3.2	18

135	Toxicants in cigarette smoke adsorbed on red phosphorene nanosheet: A first-principles insight. *Chemical Physics*, **2020**, 530, 110604	2.3	18
134	Molecular interaction studies of cumene and toluene on arsenene nanosheet a first-principles outlook. *Molecular Physics*, **2021**, 119, e1800853	1.7	18
133	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
132	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
131	Investigation on probing explosive nitroaromatic compound vapors using graphyne nanosheet: a first-principle study. *Structural Chemistry*, **2019**, 30, 657-667	1.8	17
130	Square-octagon arsenene nanosheet as chemical nanosensor for M-xylene and toluene A DFT outlook. *Computational and Theoretical Chemistry*, **2021**, 1196, 113088	2	17
129	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
128	Switching properties of quinquephenylene molecular device A first-principles approach. *Chemical Physics Letters*, **2017**, 675, 131-136	2.5	16
127	First-principles studies on transport property and adsorption characteristics of trimethylamine on MoO3 molecular device. *Chemical Physics Letters*, **2015**, 641, 129-135	2.5	16
126	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
125	Influence of fluorine substitution on the properties of CdO nanocluster : a DFT approach. *Structural Chemistry*, **2014**, 25, 389-401	1.8	16
124	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
123	First-Principles Insights of CO Adsorption Characteristics on Ge and In Substituted Silicene Nanosheet. *Silicon*, **2017**, 9, 327-337	2.4	15
122	Interaction studies of volatiles from jackfruit on phosphorene nanosheet DFT outlook. *Structural Chemistry*, **2020**, 31, 1851-1860	1.8	15
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118	DFT investigation on structural stability, electronic properties and CO adsorption characteristics on anatase and rutile TiO 2 nanostructures. *Ceramics International*, **2014**, 40, 16147-16158	5.1	15

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116	Physical Properties of Spray Deposited Mg Doped CdO Thin Films. *Journal of Applied Sciences*, **2012**, 12, 1754-1757	0.3	15
115	Explosive vapor detection using novel graphdiyne nanoribbons: first-principles investigation. *Structural Chemistry*, **2020**, 31, 709-717	1.8	15
114	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
113	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
112	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
111	Adsorption studies of nucleobases on arsenene nanosheet based on first-principles research. *Journal of Molecular Graphics and Modelling*, **2021**, 103, 107827	2.8	15
110	Alcohol molecular interaction studies on stair phosphorene nanosheets: a first-principles approach. *Structural Chemistry*, **2021**, 32, 27-36	1.8	15
109	Adsorption behaviour of trichloropropane and tetrachloroethylene on phosphorene sheets: A first-principles insight. *Computational and Theoretical Chemistry*, **2021**, 1203, 113347	2	15
108	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
107	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
106	Exploring electronic transport properties of AlN nanoribbon molecular device A first-principles investigation. *Solid State Sciences*, **2015**, 39, 45-51	3.4	14
105	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
104	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
103	DFT investigation of NH3 gas interactions on TeO2 nanostructures. *Progress in Natural Science: Materials International*, **2016**, 26, 129-138	3.6	14
102	Nucleobases adsorption studies on silicane layer: A first-principles investigation. *Journal of Molecular Graphics and Modelling*, **2018**, 85, 48-55	2.8	14
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100	FIRST-PRINCIPLES INVESTIGATION ON BAND STRUCTURE AND ELECTRONIC TRANSPORT PROPERTY OF GALLIUM NITRIDE NANORIBBON. *Nano*, **2014**, 09, 1450020	1.1	14

99	Investigation on the structural stability and electronic properties of InSb nanostructures A DFT approach. *AEJ - Alexandria Engineering Journal*, **2014**, 53, 437-444	6.1	14
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97	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
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94	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
93	Adsorption behaviour of sulfisoxazole molecules on tricycle arsenene nanoribbon - a first-principles study. *Journal of Molecular Liquids*, **2021**, 343, 117635	6	14
92	Novel arsenene nanosheets for sensing toxic malathion and parathion A first-principles approach. *Computational and Theoretical Chemistry*, **2020**, 1190, 112995	2	13
91	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
90	Electronic transport properties and CO adsorption characteristics on TiO2 molecular device A first-principles study. *Microelectronic Engineering*, **2016**, 162, 51-56	2.5	13
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87	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
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85	Interaction Studies of Methanol and Ethanol Vapors on Green Phosphorene Sheets: A First-Principles Study. *ChemistrySelect*, **2019**, 4, 14237-14243	1.8	13
84	Surface assimilation studies of ethyl methyl sulfide on gamma phosphorene sheets a DFT outlook. *Molecular Physics*, **2020**, 118, e1774089	1.7	12
83	Band structure and transport studies on impurity substituted InSe nanosheet A first-principles investigation. *Superlattices and Microstructures*, **2015**, 79, 135-147	2.8	12
82	Dimethyl and ethyl methyl ether adsorption studies on antimonene nanosheets a first-principles study. *Molecular Simulation*, **2020**, 46, 1354-1361	2	12

81	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
80	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
79	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
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77	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
76	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
75	Band structure and transport studies on InP nanotube A first-principles investigation. *Superlattices and Microstructures*, **2015**, 83, 193-209	2.8	11
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72	Quantum chemical studies on (ZnO)n/(NiO)n heterostructured nanoclusters. *Molecular Physics*, **2014**, 112, 151-164	1.7	11
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70	Chemosensing nature of black phosphorene nanotube towards C14H9Cl5 and C10H5Cl7 molecules A first-principles insight. *Computational and Theoretical Chemistry*, **2021**, 1196, 113109	2	11
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68	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
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