Ali Ahmadi

List of Publications by Citations

136 papers	7,168 citations	58 h-index	80 g-index
138 ext. papers	7,948 ext. citations	2.8 avg, IF	6.56 L-index

#	Paper	IF	Citations
136	Theoretical Study on the Al-Doped ZnO Nanoclusters for CO Chemical Sensors. *Journal of Physical Chemistry C*, **2015**, 119, 6398-6404	3.8	265
135	Detection of phosgene by Sc-doped BN nanotubes: A DFT study. *Sensors and Actuators B: Chemical*, **2012**, 171-172, 846-852	8.5	240
134	Theoretical study of aluminum nitride nanotubes for chemical sensing of formaldehyde. *Sensors and Actuators B: Chemical*, **2012**, 161, 1025-1029	8.5	203
133	Effects of Al Doping and Double-Antisite Defect on the Adsorption of HCN on a BC2N Nanotube: Density Functional Theory Studies. *Journal of Physical Chemistry C*, **2013**, 117, 2427-2432	3.8	176
132	DFT study of NH3 adsorption on pristine, Ni- and Si-doped graphynes. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2014**, 378, 2184-2190	2.3	169
131	Sensing behavior of Al and Si doped BC3 graphenes to formaldehyde. *Sensors and Actuators B: Chemical*, **2013**, 181, 829-834	8.5	158
130	Al-doped graphene-like BN nanosheet as a sensor for para-nitrophenol: DFT study. *Superlattices and Microstructures*, **2013**, 59, 115-122	2.8	151
129	Response of Si- and Al-doped graphenes toward HCN: A computational study. *Applied Surface Science*, **2013**, 265, 412-417	6.7	130
128	A comparative study on the B12N12, Al12N12, B12P12 and Al12P12 fullerene-like cages. *Journal of Molecular Modeling*, **2012**, 18, 2653-8	2	129
127	Theoretical study of CO adsorption on the surface of BN, AlN, BP and AlP nanotubes. *Surface Science*, **2012**, 606, 981-985	1.8	125
126	A first-principles study of the adsorption behavior of CO on Al- and Ga-doped single-walled BN nanotubes. *Applied Surface Science*, **2013**, 270, 25-32	6.7	116
125	Selective function of Al12N12 nano-cage towards NO and CO molecules. *Computational Materials Science*, **2012**, 62, 71-74	3.2	113
124	Sensing behavior of BN nanosheet toward nitrous oxide: A DFT study. *Chinese Chemical Letters*, **2015**, 26, 1042-1045	8.1	112
123	Sensing properties of BN nanotube toward carcinogenic 4-chloroaniline: A computational study. *Physica E: Low-Dimensional Systems and Nanostructures*, **2016**, 76, 6-11	3	110
122	Toxic CO detection by B12N12 nanocluster. *Microelectronics Journal*, **2011**, 42, 1400-1403	1.8	103
121	H2O2 adsorption on the BN and SiC nanotubes: A DFT study. *Physica E: Low-Dimensional Systems and Nanostructures*, **2013**, 48, 176-180	3	100
120	A DFT study on the functionalization of a BN nanosheet with PCX, (PC=phenyl carbamate, X=OCH3, CH3, NH2, NO2 and CN). *Applied Surface Science*, **2013**, 268, 436-441	6.7	100

119	B12N12 Nano-cage as Potential Sensor for NO2 Detection. *Chinese Journal of Chemical Physics*, **2012**, 25, 60-64	0.9	100
118	NO2 detection by nanosized AlN sheet in the presence of NH3: DFT studies. *Applied Surface Science*, **2013**, 274, 217-220	6.7	97
117	Adsorption and dissociation of Cl2 molecule on ZnO nanocluster. *Applied Surface Science*, **2012**, 258, 8171-8176	6.7	95
116	Computational study of CO and NO adsorption on magnesium oxide nanotubes. *Physica E: Low-Dimensional Systems and Nanostructures*, **2011**, 44, 546-549	3	88
115	Quantum chemical study of fluorinated AlN nano-cage. *Applied Surface Science*, **2012**, 259, 631-636	6.7	86
114	Interaction of small molecules (NO, H2, N2, and CH4) with BN nanocluster surface. *Structural Chemistry*, **2012**, 23, 1567-1572	1.8	86
113	AlN nanotube as a potential electronic sensor for nitrogen dioxide. *Microelectronics Journal*, **2012**, 43, 452-455	1.8	84
112	Chemisorption of NH3 at the open ends of boron nitride nanotubes: a DFT study. *Structural Chemistry*, **2011**, 22, 183-188	1.8	84
111	A first-principles study of H2S adsorption and dissociation on the AlN nanotube. *Physica E: Low-Dimensional Systems and Nanostructures*, **2012**, 44, 1963-1968	3	83
110	Theoretical study of hydrogen adsorption on the B12P12 fullerene-like nanocluster. *Computational Materials Science*, **2012**, 54, 115-118	3.2	83
109	The H2 dissociation on the BN, AlN, BP and AlP nanotubes: a comparative study. *Journal of Molecular Modeling*, **2012**, 18, 2343-8	2	80
108	Carbon nitride nanotube as a sensor for alkali and alkaline earth cations. *Applied Surface Science*, **2013**, 264, 699-706	6.7	80
107	B-doping makes the carbon nanocones sensitive towards NO molecules. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2012**, 377, 107-111	2.3	79
106	Functionalization of BN nanosheet with N2H4 may be feasible in the presence of Stone□Wales defect. *Structural Chemistry*, **2013**, 24, 1565-1570	1.8	78
105	DFT study on the functionalization of a BN nanotube with sulfamide. *Applied Surface Science*, **2013**, 266, 182-187	6.7	78
104	Can aluminum nitride nanotubes detect the toxic NH3 molecules?. *Physica E: Low-Dimensional Systems and Nanostructures*, **2012**, 44, 1357-1360	3	78
103	Ab initio study of NH3 and H2O adsorption on pristine and Na-doped MgO nanotubes. *Structural Chemistry*, **2013**, 24, 165-170	1.8	76
102	Interaction of NH3 with aluminum nitride nanotube: Electrostatic vs. covalent. *Physica E: Low-Dimensional Systems and Nanostructures*, **2011**, 43, 1717-1719	3	76

101	DNA nucleobase interaction with graphene like BC3 nano-sheet based on density functional theory calculations. *Thin Solid Films*, **2015**, 589, 52-56	2.2	74
100	A theoretical study of CO adsorption on aluminum nitride nanotubes. *Structural Chemistry*, **2012**, 23, 653-657	1.8	74
99	Ab initio studies of the interaction of formaldehyde with beryllium oxide nanotube. *Physica E: Low-Dimensional Systems and Nanostructures*, **2015**, 68, 22-27	3	73
98	A large gap opening of graphene induced by the adsorption of CO on the Al-doped site. *Journal of Molecular Modeling*, **2013**, 19, 3007-14	2	72
97	Benchmarking of ONIOM method for the study of NH3 dissociation at open ends of BNNTs. *Journal of Molecular Modeling*, **2012**, 18, 1729-34	2	71
96	Adsorption of carbon monoxide on the pristine, B- and Al-doped C3N nanosheets. *Journal of Molecular Modeling*, **2015**, 21, 116	2	70
95	Cation-□interaction of alkali metal ions with C24 fullerene: a DFT study. *Journal of Molecular Modeling*, **2012**, 18, 3535-40	2	70
94	Electronic sensor for sulfide dioxide based on AlN nanotubes: a computational study. *Journal of Molecular Modeling*, **2012**, 18, 4745-50	2	70
93	DFT studies of Si- and Al-doping effects on the acetone sensing properties of BC3 graphene. *Molecular Physics*, **2013**, 111, 3320-3326	1.7	66
92	A computational study of AlN nanotube as an oxygen detector. *Chinese Chemical Letters*, **2012**, 23, 965-968	1.8	66
91	Nitrate adsorption by carbon nanotubes in the vacuum and aqueous phase. *Monatshefte F□ Chemie* , **2012**, 143, 1623-1626	1.4	65
90	DFT study of NO2 adsorption on the AlN nanocones. *Computational and Theoretical Chemistry*, **2013** , 1008, 20-26	2	64
89	Hydrogen dissociation on diene-functionalized carbon nanotubes. *Journal of Molecular Modeling*, **2013**, 19, 255-61	2	63
88	The effect of surface curvature of aluminum nitride nanotubes on the adsorption of NH3. *Structural Chemistry*, **2011**, 22, 1261-1265	1.8	63
87	The alkali and alkaline earth metal doped ZnO nanotubes: DFT studies. *Physica B: Condensed Matter* , **2014**, 432, 105-110	2.8	62
86	F□Cl□Li+ and Na+ adsorption on AlN nanotube surface: A DFT study. *Physica E: Low-Dimensional Systems and Nanostructures*, **2015**, 69, 75-80	3	62
85	Density-functional calculations of HCN adsorption on the pristine and Si-doped graphynes. *Structural Chemistry*, **2014**, 25, 1-7	1.8	62
84	Ammonia monitoring by carbon nitride nanotubes: A density functional study. *Thin Solid Films*, **2013** , 534, 650-654	2.2	62

83	Theoretical investigation of C60 fullerene functionalization with tetrazine. *Computational and Theoretical Chemistry*, **2012**, 992, 164-167	2	61
82	Phenol adsorption study on pristine, Ga-, and In-doped (4,4) armchair single-walled boron nitride nanotubes. *Computational and Theoretical Chemistry*, **2012**, 997, 63-69	2	60
81	Carbon nanocone as an ammonia sensor: DFT studies. *Structural Chemistry*, **2013**, 24, 1099-1103	1.8	58
80	Sensing behavior of Al-rich AlN nanotube toward hydrogen cyanide. *Journal of Molecular Modeling*, **2013**, 19, 2197-203	2	58
79	Carbon nanotube functionalization with carboxylic derivatives: a DFT study. *Journal of Molecular Modeling*, **2013**, 19, 391-6	2	58
78	Functionalization of [60] fullerene with butadienes: A DFT study. *Applied Surface Science*, **2012**, 258, 8980-8984	6.7	55
77	Effect of electrostatic interaction on the methylene blue and methyl orange adsorption by the pristine and functionalized carbon nanotubes. *Physica E: Low-Dimensional Systems and Nanostructures*, **2016**, 83, 1-6	3	55
76	ZnO Nanocluster as a Potential Catalyst for Dissociation of H2S Molecule. *Journal of Cluster Science*, **2013**, 24, 341-347	3	54
75	A DFT study on the sensing behavior of a BC2N nanotube toward formaldehyde. *Journal of Molecular Modeling*, **2013**, 19, 3843-50	2	46
74	DFT study of the dissociative adsorption of HF on an AlN nanotube. *Comptes Rendus Chimie*, **2013**, 16, 985-989	2.7	46
73	Structural and electronic properties of pyrrolidine-functionalized [60]fullerenes. *Journal of Physics and Chemistry of Solids*, **2013**, 74, 1594-1598	3.9	45
72	Theoretical study of carbonyl sulfide adsorption on Ag-doped SiC nanotubes. *Journal of the Iranian Chemical Society*, **2015**, 12, 1071-1076	2	39
71	Density functional study on the adsorption and dissociation of nitroamine over the nanosized tube of MgO. *Physica E: Low-Dimensional Systems and Nanostructures*, **2014**, 62, 48-54	3	38
70	Adsorption of H2S at Stone□Wales defects of graphene-like BC3: a computational study. *Molecular Physics*, **2014**, 112, 2737-2745	1.7	38
69	The electronic response of nano-sized tube of BeO to CO molecule: a density functional study. *Structural Chemistry*, **2015**, 26, 809-814	1.8	38
68	Tuning the electronic properties of C30B15N15 fullerene via encapsulation of alkali and alkali earth metals. *Synthetic Metals*, **2013**, 177, 94-99	3.6	34
67	Hydrogen peroxide reduction in the oxygen vacancies of ZnO nanotubes. *Thin Solid Films*, **2014**, 556, 566-570	2.2	34
66	Role of sodium decoration on the methane storage properties of BC3 nanosheet. *Structural Chemistry*, **2014**, 25, 1083-1090	1.8	34

65	Energetic, structural, and electronic properties of hydrogenated Al12P12 nanocluster. *Physica E: Low-Dimensional Systems and Nanostructures*, **2012**, 44, 1436-1440	3	34
64	Multivalent calix[4]arene-based fluorescent sensor for detecting silver ions in aqueous media and physiological environment. *Biosensors and Bioelectronics*, **2017**, 90, 290-297	11.8	33
63	Formaldehyde adsorption on the interior and exterior surfaces of CN nanotubes. *Structural Chemistry*, **2013**, 24, 1331-1337	1.8	33
62	First-principle study of methanol adsorption on Ni (Pd)-decorated graphene. *Journal of the Iranian Chemical Society*, **2015**, 12, 751-756	2	32
61	Adsorption of Formic Acid and Formate Anion on ZnO Nanocage: A DFT Study. *Journal of Cluster Science*, **2015**, 26, 609-621	3	32
60	A density functional study on the acidity properties of pristine and modified SiC nano-sheets. *Physica B: Condensed Matter*, **2014**, 443, 54-59	2.8	32
59	Selective detection of F2 in the presence of CO, N2, O2, and H2 molecules using a ZnO nanocluster. *Monatshefte Fü Chemie*, **2015**, 146, 1233-1239	1.4	30
58	Transition metal atom adsorptions on a boron nitride nanocage. *Structural Chemistry*, **2013**, 24, 1039-1044	1.8	28
57	Ammonia borane reaction with a BN nanotube: a hydrogen storage route. *Monatshefte Fü Chemie*, **2014**, 145, 1083-1087	1.4	27
56	Electronic, energetic, and structural properties of C- and Si-doped Mg12O12 nano-cages. *Computational Materials Science*, **2013**, 79, 352-355	3.2	27
55	Adsorption of CO molecule on AlN nanotubes by parallel electric field. *Journal of Molecular Modeling*, **2013**, 19, 859-70	2	27
54	Exohedral and endohedral adsorption of alkaline earth cations in BN nanocluster. *Journal of Molecular Modeling*, **2013**, 19, 1445-50	2	27
53	Theoretical Study of Thiazole Adsorption on the (6,0) zigzag Single-Walled Boron Nitride Nanotube. *Bulletin of the Korean Chemical Society*, **2012**, 33, 3285-3292	1.2	27
52	Arsenic interactions with a fullerene-like BN cage in the vacuum and aqueous phase. *Journal of Molecular Modeling*, **2013**, 19, 833-7	2	26
51	Nitrous oxide adsorption on pristine and Si-doped AlN nanotubes. *Journal of Molecular Modeling*, **2013**, 19, 943-9	2	26
50	A density functional theory study on acetylene-functionalized BN nanotubes. *Structural Chemistry*, **2013**, 24, 1007-1013	1.8	26
49	Hydrogen fluoride on the pristine, Al and Si doped BC2N nanotubes: A computational study. *Computational Materials Science*, **2014**, 82, 197-201	3.2	25
48	A DFT Study on CO2Interaction with a BN Nano-Cage. *Bulletin of the Korean Chemical Society*, **2012**, 33, 3338-3342	1.2	25

47	Influence of antisite defect upon decomposition of nitrous oxide over graphene-analogue SiC. *Thin Solid Films*, **2014**, 552, 111-115	2.2	24
46	Methanol-sensing characteristics of zinc oxide nanotubes: quantum chemical study. *Monatshefte Fü Chemie*, **2014**, 145, 1253-1257	1.4	21
45	Working Mechanism of a BC 3 Nanotube Carbon Monoxide Gas Sensor. *Communications in Theoretical Physics*, **2013**, 60, 113-118	2.4	21
44	Electronic Response of Nano-sized Cages of ZnO and MgO to Presence of Nitric Oxide. *Chinese Journal of Chemical Physics*, **2013**, 26, 231-236	0.9	21
43	First Principles Study on Encapsulation of Alkali Metals into ZnO Nanocage. *Chinese Journal of Chemical Physics*, **2012**, 25, 671-675	0.9	21
42	Selective adsorption behavior of BC2N nanotubes toward fluoride and chloride. *Solid State Communications*, **2013**, 159, 8-12	1.6	20
41	DFT studies of Hydrogen adsorption and dissociation on MgO nanotubes. *Main Group Chemistry*, **2016**, 15, 107-116	0.6	20
40	NH3 on a BC3 nanotube: effect of doping and decoration of aluminum. *Journal of Molecular Modeling*, **2013**, 19, 3793-8	2	19
39	Quantum chemical analysis on hydrogenated Zn12O12 nanoclusters. *Comptes Rendus Chimie*, **2013**, 16, 122-128	2.7	19
38	Fluorination of the exterior surface of AlN nanotube: A DFT study. *Superlattices and Microstructures* , **2013**, 53, 9-15	2.8	19
37	Electronic response of BC3 nanotube to CS2 molecules: DFT studies. *Computational and Theoretical Chemistry*, **2013**, 1008, 1-7	2	18
36	Co-adsorption of CO molecules at the open ends of MgO nanotubes. *Structural Chemistry*, **2012**, 23, 1981-1986	1.8	18
35	Functionalization of the pristine and stone-wales defected BC3 graphenes with pyrene. *Journal of Molecular Modeling*, **2014**, 20, 2539	2	17
34	Aluminum nitride nanotubes. *Chemical Papers*, **2017**, 71, 881-893	1.9	16
33	Theoretical Study of Phenol Adsorption on Pristine, Ga-Doped, and Pd-Decorated (6,0) Zigzag Single-Walled Boron Phosphide Nanotubes. *Journal of Cluster Science*, **2013**, 24, 49-60	3	16
32	Capture of carbon dioxide by a nanosized tube of BeO: a DFT study. *Structural Chemistry*, **2014**, 25, 419-428	1.8	16
31	Effect of Gallium Doping on Electronic and Structural Properties (6,0) Zigzag Silicon Carbide Nanotube as a p-Semiconductor. *Journal of Cluster Science*, **2012**, 23, 1119-1132	3	16
30	DFT study of ozone dissociation on BC graphene with Stone-Wales defects. *Journal of Molecular Modeling*, **2014**, 20, 2071	2	15

29	Fluorination of BC3 nanotubes: DFT studies. *Journal of Molecular Modeling*, **2013**, 19, 3941-6	2	15
28	Adsorption of nitrous oxide on the (6,0) magnesium oxide nanotube. *Chinese Chemical Letters*, **2012**, 23, 1275-1278	8.1	15
27	First Principles Calculations of Electric Field Effect on the (6,0) Zigzag Single-Walled Silicon Carbide Nanotube for use in Nano-Electronic Circuits. *Journal of Cluster Science*, **2013**, 24, 591-604	3	14
26	Theoretical study of cyano radical adsorption on (6,0) zigzag single-walled carbon nanotube. *Monatshefte F□ Chemie*, **2012**, 143, 1463-1470	1.4	14
25	The Alkali Metal Interactions with MgO Nanotubes. *Bulletin of the Korean Chemical Society*, **2012**, 33, 1925-1928	1.2	14
24	Au-decorated BN nanotube as a breathalyzer for potential medical applications. *Journal of Molecular Liquids*, **2020**, 312, 113454	6	12
23	Exohedral functionalization of C60 by [4+2] cycloaddition of multiple anthracenes. *Structural Chemistry*, **2014**, 25, 785-791	1.8	12
22	First-principles calculations of structural stability, electronic, and electrical responses of GeC nanotube under electric field effect for use in nanoelectronic devices. *Superlattices and Microstructures*, **2012**, 52, 1119-1130	2.8	12
21	Electronic, Energetic, and Geometric Properties of Methylene-Functionalized C60. *Journal of Cluster Science*, **2013**, 24, 669-678	3	12
20	Electric field effect on the zigzag (6,0) single-wall BC2N nanotube for use in nano-electronic circuits. *Journal of Molecular Modeling*, **2013**, 19, 97-107	2	11
19	Decomposition of methanol on nanosized tube of magnesium oxide: A theoretical study. *Computational Materials Science*, **2013**, 79, 182-186	3.2	11
18	Adsorption of Na, Mg, and Al atoms on BN nanotubes. *Thin Solid Films*, **2012**, 526, 139-142	2.2	11
17	A theoretical study on surface modification of a nanosized BC3 tube using C2H4 and its derivatives. *Structural Chemistry*, **2014**, 25, 221-229	1.8	10
16	Electric field effect on (6,0) zigzag single-walled aluminum nitride nanotube. *Journal of Molecular Modeling*, **2012**, 18, 4477-89	2	10
15	Theoretical study on the functionalization of BC□N nanotube with amino groups. *Journal of Molecular Modeling*, **2013**, 19, 2211-6	2	10
14	Covalent functionalization of AlN nanotubes with acetylene. *Physica E: Low-Dimensional Systems and Nanostructures*, **2013**, 47, 147-151	3	8
13	DFT study on [4+2] and [2+2] cycloadditions to [60] fullerene. *Chemical Papers*, **2014**, 68,	1.9	8
12	Adsorption and Electronic Structure Study of Imidazole on (6,0) Zigzag Single-Walled Boron Nitride Nanotube. *Journal of Cluster Science*, **2012**, 24, 31	3	8

11	A Theoretical Study of OH and OCH3 Free Radical Adsorption on a Nanosized Tube of BC2N. *Journal of Cluster Science*, **2013**, 24, 1011-1020	3	6
10	Electronic structure study of Si-doped (4,4) armchair single-walled boron phosphide nanotube as a semiconductor. *Monatshefte F□ Chemie*, **2012**, 143, 1627-1635	1.4	6
9	The influence of Stone-Wales defects in nanographene on the performance of Na-ion batteries. *Journal of Molecular Graphics and Modelling*, **2020**, 98, 107578	2.8	5
8	Adsorption of Thiophene on Aluminum Nitride Nanotubes. *Phosphorus, Sulfur and Silicon and the Related Elements*, **2013**, 188, 1172-1177	1	5
7	Density Functional Study of the Adsorption of Methanol and its Derivatives on Boron Nitride Nanotubes. *Adsorption Science and Technology*, **2013**, 31, 767-776	3.6	4
6	Application of hexa-peri-hexabenzocoronene nanographene and its B, N, and Bn doped forms in Na-ion batteries: A density functional theory study. *Thin Solid Films*, **2020**, 704, 137979	2.2	3
5	Explosive properties of nanosized diacetone diperoxide and its nitro derivatives: a DFT study. *Monatshefte F□ Chemie*, **2015**, 146, 1401-1408	1.4	3
4	Role of Diameter, Model, and Length of Boron Nitride Nanotubes in Adsorption of Formaldehyde. *Fullerenes Nanotubes and Carbon Nanostructures*, **2015**, 23, 62-67	1.8	1
3	Surface Modification of Carbon Nanotubes with Nitrenes: A DFT Study. *Fullerenes Nanotubes and Carbon Nanostructures*, **2015**, 23, 326-331	1.8	1
2	NMR and NQR study of Si-doped (6,0) zigzag single-walled aluminum nitride nanotube as n or P-semiconductors. *Journal of Molecular Modeling*, **2012**, 18, 4427-36	2	1
1	Theoretical Study of Arsenic-Doped (6,0) Zigzag Silicon Carbide Nanotube as a N-Semiconductor. *Phosphorus, Sulfur and Silicon and the Related Elements*, **2013**, 188, 1382-1393	1	0