Ali Ahmadi

List of Publications by Year
in descending order

136	8,703	18482 62	48315 88
papers	citations	h-index	g-index

138	138	138	2352
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Theoretical Study on the Al-Doped ZnO Nanoclusters for CO Chemical Sensors. Journal of Physical Chemistry C, 2015, 119, 6398-6404.	3.1	365
2	Detection of phosgene by Sc-doped BN nanotubes: A DFT study. Sensors and Actuators B: Chemical, 2012, 171-172, 846-852.	7.8	292
3	Theoretical study of aluminum nitride nanotubes for chemical sensing of formaldehyde. Sensors and Actuators B: Chemical, 2012, 161, 1025-1029.	7.8	248
4	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.	3.1	219
5	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.	2.1	198
6	Sensing behavior of Al and Si doped BC3 graphenes to formaldehyde. Sensors and Actuators B: Chemical, 2013, 181, 829-834.	7.8	188
7	Al-doped graphene-like BN nanosheet as a sensor for para-nitrophenol: DFT study. Superlattices and Microstructures, 2013, 59, 115-122.	3.1	185
8	A comparative study on the B12N12, Al12N12, B12P12 and Al12P12 fullerene-like cages. Journal of Molecular Modeling, 2012, 18, 2653-2658.	1.8	160
9	Theoretical study of CO adsorption on the surface of BN, AlN, BP and AlP nanotubes. Surface Science, 2012, 606, 981-985.	1.9	152
10	Response of Si- and Al-doped graphenes toward HCN: A computational study. Applied Surface Science, 2013, 265, 412-417.	6.1	151
11	Sensing behavior of BN nanosheet toward nitrous oxide: A DFT study. Chinese Chemical Letters, 2015, 26, 1042-1045.	9.0	137
12	Selective function of Al12N12 nano-cage towards NO and CO molecules. Computational Materials Science, 2012, 62, 71-74.	3.0	136
13	A DFT study on the functionalization of a BN nanosheet with PCX, (PC=phenyl carbamate, X=OCH3, CH3,) Tj ETQq1 1 0.784314 rgBT /C	6.1	136
14	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.	6.1	135
15	Sensing properties of BN nanotube toward carcinogenic 4-chloroaniline: A computational study. Physica E: Low-Dimensional Systems and Nanostructures, 2016, 76, 6-11.	2.7	131
16	B12N12 Nano-cage as Potential Sensor for NO2 Detection. Chinese Journal of Chemical Physics, 2012, 25, 60-64.	1.3	126
17	Toxic CO detection by B12N12 nanocluster. Microelectronics Journal, 2011, 42, 1400-1403.	2.0	124
18	Adsorption and dissociation of Cl2 molecule on ZnO nanocluster. Applied Surface Science, 2012, 258, 8171-8176.	6.1	117

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19	NO2 detection by nanosized AlN sheet in the presence of NH3: DFT studies. Applied Surface Science, 2013, 274, 217-220.	6.1	117
20	H2O2 adsorption on the BN and SiC nanotubes: A DFT study. Physica E: Low-Dimensional Systems and Nanostructures, 2013, 48, 176-180.	2.7	114
21	The H2 dissociation on the BN, AlN, BP and AlP nanotubes: a comparative study. Journal of Molecular Modeling, 2012, 18, 2343-2348.	1.8	111
22	Ab initio studies of the interaction of formaldehyde with beryllium oxide nanotube. Physica E: Low-Dimensional Systems and Nanostructures, 2015, 68, 22-27.	2.7	106
23	B-doping makes the carbon nanocones sensitive towards NO molecules. Physics Letters, Section A: General, Atomic and Solid State Physics, 2012, 377, 107-111.	2.1	105
24	Interaction of small molecules (NO, H2, N2, and CH4) with BN nanocluster surface. Structural Chemistry, 2012, 23, 1567-1572.	2.0	103
25	Computational study of CO and NO adsorption on magnesium oxide nanotubes. Physica E: Low-Dimensional Systems and Nanostructures, 2011, 44, 546-549.	2.7	100
26	Quantum chemical study of fluorinated AlN nano-cage. Applied Surface Science, 2012, 259, 631-636.	6.1	97
27	AlN nanotube as a potential electronic sensor for nitrogen dioxide. Microelectronics Journal, 2012, 43, 452-455.	2.0	96
28	Theoretical study of hydrogen adsorption on the B12P12 fullerene-like nanocluster. Computational Materials Science, 2012, 54, 115-118.	3.0	95
29	A first-principles study of H2S adsorption and dissociation on the AlN nanotube. Physica E: Low-Dimensional Systems and Nanostructures, 2012, 44, 1963-1968.	2.7	92
30	Chemisorption of NH3 at the open ends of boron nitride nanotubes: a DFT study. Structural Chemistry, 2011, 22, 183-188.	2.0	88
31	DNA nucleobase interaction with graphene like BC3 nano-sheet based on density functional theory calculations. Thin Solid Films, 2015, 589, 52-56.	1.8	88
32	DFT study on the functionalization of a BN nanotube with sulfamide. Applied Surface Science, 2013, 266, 182-187.	6.1	87
33	Functionalization of BN nanosheet with N2H4 may be feasible in the presence of Stoneâ€“Wales defect. Structural Chemistry, 2013, 24, 1565-1570.	2.0	86
34	Can aluminum nitride nanotubes detect the toxic NH3 molecules?. Physica E: Low-Dimensional Systems and Nanostructures, 2012, 44, 1357-1360.	2.7	85
35	Interaction of NH3 with aluminum nitride nanotube: Electrostatic vs. covalent. Physica E: Low-Dimensional Systems and Nanostructures, 2011, 43, 1717-1719.	2.7	84
36	Carbon nitride nanotube as a sensor for alkali and alkaline earth cations. Applied Surface Science, 2013, 264, 699-706.	6.1	82

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37	Cation-Ï€ interaction of alkali metal ions with C24 fullerene: a DFT study. Journal of Molecular Modeling, 2012, 18, 3535-3540.	1.8	81
38	A large gap opening of graphene induced by the adsorption of CO on the Al-doped site. Journal of Molecular Modeling, 2013, 19, 3007-3014.	1.8	81
39	The alkali and alkaline earth metal doped ZnO nanotubes: DFT studies. Physica B: Condensed Matter, 2014, 432, 105-110.	2.7	81
40	Electronic sensor for sulfide dioxide based on AlN nanotubes: a computational study. Journal of Molecular Modeling, 2012, 18, 4745-4750.	1.8	80
41	Ab initio study of NH3 and H2O adsorption on pristine and Na-doped MgO nanotubes. Structural Chemistry, 2013, 24, 165-170.	2.0	80
42	Density-functional calculations of HCN adsorption on the pristine and Si-doped graphynes. Structural Chemistry, 2014, 25, 1-7.	2.0	79
43	A theoretical study of CO adsorption on aluminum nitride nanotubes. Structural Chemistry, 2012, 23, 653-657.	2.0	77
44	DFT study of NO2 adsorption on the AlN nanocones. Computational and Theoretical Chemistry, 2013, 1008, 20-26.	2.5	77
45	DFT studies of Si- and Al-doping effects on the acetone sensing properties of BC₃ graphene. Molecular Physics, 2013, 111, 3320-3326.	1.7	77
46	A computational study of AlN nanotube as an oxygen detector. Chinese Chemical Letters, 2012, 23, 965-968.	9.0	76
47	Fâ^', Clâ^', Li+ and Na+ adsorption on AlN nanotube surface: A DFT study. Physica E: Low-Dimensional Systems and Nanostructures, 2015, 69, 75-80.	2.7	76
48	Theoretical study of carbonyl sulfide adsorption on Ag-doped SiC nanotubes. Journal of the Iranian Chemical Society, 2015, 12, 1071-1076.	2.2	76
49	Benchmarking of ONIOM method for the study of NH3 dissociation at open ends of BNNTs. Journal of Molecular Modeling, 2012, 18, 1729-1734.	1.8	75
50	Ammonia monitoring by carbon nitride nanotubes: A density functional study. Thin Solid Films, 2013, 534, 650-654.	1.8	75
51	Adsorption of carbon monoxide on the pristine, B- and Al-doped C3N nanosheets. Journal of Molecular Modeling, 2015, 21, 116.	1.8	74
52	Theoretical investigation of C60 fullerene functionalization with tetrazine. Computational and Theoretical Chemistry, 2012, 992, 164-167.	2.5	73
53	The effect of surface curvature of aluminum nitride nanotubes on the adsorption of NH3. Structural Chemistry, 2011, 22, 1261-1265.	2.0	72
54	Hydrogen dissociation on diene-functionalized carbon nanotubes. Journal of Molecular Modeling, 2013, 19, 255-261.	1.8	72

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55	Carbon nanocone as an ammonia sensor: DFT studies. Structural Chemistry, 2013, 24, 1099-1103.	2.0	71
56	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.	2.5	70
57	Structural and electronic properties of pyrrolidine-functionalized [60]fullerenes. Journal of Physics and Chemistry of Solids, 2013, 74, 1594-1598.	4.0	70
58	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.	2.7	69
59	Nitrate adsorption by carbon nanotubes in the vacuum and aqueous phase. Monatshefte FÃ¼r Chemie, 2012, 143, 1623-1626.	1.8	68
60	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.	2.7	64
61	ZnO Nanocluster as a Potential Catalyst for Dissociation of H2S Molecule. Journal of Cluster Science, 2013, 24, 341-347.	3.3	63
62	A DFT study on the sensing behavior of a BC2N nanotube toward formaldehyde. Journal of Molecular Modeling, 2013, 19, 3843-3850.	1.8	63
63	Sensing behavior of Al-rich AlN nanotube toward hydrogen cyanide. Journal of Molecular Modeling, 2013, 19, 2197-2203.	1.8	63
64	Carbon nanotube functionalization with carboxylic derivatives: a DFT study. Journal of Molecular Modeling, 2013, 19, 391-396.	1.8	63
65	Functionalization of [60] fullerene with butadienes: A DFT study. Applied Surface Science, 2012, 258, 8980-8984.	6.1	59
66	Adsorption of H₂S at Stoneâ€“Wales defects of graphene-like BC₃: a computational study. Molecular Physics, 2014, 112, 2737-2745.	1.7	59
67	DFT study of the dissociative adsorption of HF on an AlN nanotube. Comptes Rendus Chimie, 2013, 16, 985-989.	0.5	58
68	Aluminum nitride nanotubes. Chemical Papers, 2017, 71, 881-893.	2.2	51
69	Multivalent calix[4]arene-based fluorescent sensor for detecting silver ions in aqueous media and physiological environment. Biosensors and Bioelectronics, 2017, 90, 290-297.	10.1	47
70	The electronic response of nano-sized tube of BeO to CO molecule: a density functional study. Structural Chemistry, 2015, 26, 809-814.	2.0	44
71	Adsorption of Formic Acid and Formate Anion on ZnO Nanocage: A DFT Study. Journal of Cluster Science, 2015, 26, 609-621.	3.3	43
72	Hydrogen peroxide reduction in the oxygen vacancies of ZnO nanotubes. Thin Solid Films, 2014, 556, 566-570.	1.8	42

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73	Methanol-sensing characteristics of zinc oxide nanotubes: quantum chemical study. Monatshefte FÃ¼r Chemie, 2014, 145, 1253-1257.	1.8	40
74	First-principle study of methanol adsorption on Ni (Pd)-decorated graphene. Journal of the Iranian Chemical Society, 2015, 12, 751-756.	2.2	39
75	Energetic, structural, and electronic properties of hydrogenated Al12P12 nanocluster. Physica E: Low-Dimensional Systems and Nanostructures, 2012, 44, 1436-1440.	2.7	37
76	Tuning the electronic properties of C30B15N15 fullerene via encapsulation of alkali and alkali earth metals. Synthetic Metals, 2013, 177, 94-99.	3.9	37
77	Formaldehyde adsorption on the interior and exterior surfaces of CN nanotubes. Structural Chemistry, 2013, 24, 1331-1337.	2.0	36
78	Nitrous oxide adsorption on pristine and Si-doped AlN nanotubes. Journal of Molecular Modeling, 2013, 19, 943-949.	1.8	36
79	Role of sodium decoration on the methane storage properties of BC3 nanosheet. Structural Chemistry, 2014, 25, 1083-1090.	2.0	36
80	A density functional study on the acidity properties of pristine and modified SiC nano-sheets. Physica B: Condensed Matter, 2014, 443, 54-59.	2.7	36
81	Selective detection of F2 in the presence of CO, N2, O2, and H2 molecules using a ZnO nanocluster. Monatshefte FÃ¼r Chemie, 2015, 146, 1233-1239.	1.8	34
82	Transition metal atom adsorptions on a boron nitride nanocage. Structural Chemistry, 2013, 24, 1039-1044.	2.0	33
83	Exohedral and endohedral adsorption of alkaline earth cations in BN nanocluster. Journal of Molecular Modeling, 2013, 19, 1445-1450.	1.8	33
84	Adsorption of CO molecule on AlN nanotubes by parallel electric field. Journal of Molecular Modeling, 2013, 19, 859-870.	1.8	32
85	Decomposition of methanol on nanosized tube of magnesium oxide: A theoretical study. Computational Materials Science, 2013, 79, 182-186.	3.0	32
86	Ammonia borane reaction with a BN nanotube: a hydrogen storage route. Monatshefte FÃ¼r Chemie, 2014, 145, 1083-1087.	1.8	32
87	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.	1.9	32
88	Arsenic interactions with a fullerene-like BN cage in the vacuum and aqueous phase. Journal of Molecular Modeling, 2013, 19, 833-837.	1.8	31
89	A DFT Study on CO₂Interaction with a BN Nano-Cage. Bulletin of the Korean Chemical Society, 2012, 33, 3338-3342.	1.9	31
90	Electronic, energetic, and structural properties of C- and Si-doped Mg12O12 nano-cages. Computational Materials Science, 2013, 79, 352-355.	3.0	30

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91	Au-decorated BN nanotube as a breathalyzer for potential medical applications. Journal of Molecular Liquids, 2020, 312, 113454.	4.9	30
92	A density functional theory study on acetylene-functionalized BN nanotubes. Structural Chemistry, 2013, 24, 1007-1013.	2.0	28
93	Influence of antisite defect upon decomposition of nitrous oxide over graphene-analogue SiC. Thin Solid Films, 2014, 552, 111-115.	1.8	28
94	Electronic Response of Nano-sized Cages of ZnO and MgO to Presence of Nitric Oxide. Chinese Journal of Chemical Physics, 2013, 26, 231-236.	1.3	27
95	Hydrogen fluoride on the pristine, Al and Si doped BC2N nanotubes: A computational study. Computational Materials Science, 2014, 82, 197-201.	3.0	27
96	DFT studies of Hydrogen adsorption and dissociation on MgO nanotubes. Main Group Chemistry, 2016, 15, 107-116.	0.8	26
97	Functionalization of the pristine and stone-wales defected BC3 graphenes with pyrene. Journal of Molecular Modeling, 2014, 20, 2539.	1.8	25
98	Working Mechanism of a BC ₃ Nanotube Carbon Monoxide Gas Sensor. Communications in Theoretical Physics, 2013, 60, 113-118.	2.5	24
99	Selective adsorption behavior of BC2N nanotubes toward fluoride and chloride. Solid State Communications, 2013, 159, 8-12.	1.9	24
100	First Principles Study on Encapsulation of Alkali Metals into ZnO Nanocage. Chinese Journal of Chemical Physics, 2012, 25, 671-675.	1.3	23
101	Fluorination of BC3 nanotubes: DFT studies. Journal of Molecular Modeling, 2013, 19, 3941-3946.	1.8	23
102	Electronic response of BC3 nanotube to CS2 molecules: DFT studies. Computational and Theoretical Chemistry, 2013, 1008, 1-7.	2.5	23
103	Fluorination of the exterior surface of AlN nanotube: A DFT study. Superlattices and Microstructures, 2013, 53, 9-15.	3.1	22
104	Quantum chemical analysis on hydrogenated Zn12O12 nanoclusters. Comptes Rendus Chimie, 2013, 16, 122-128.	0.5	21
105	NH3 on a BC3 nanotube: effect of doping and decoration of aluminum. Journal of Molecular Modeling, 2013, 19, 3793-3798.	1.8	20
106	Capture of carbon dioxide by a nanosized tube of BeO: a DFT study. Structural Chemistry, 2014, 25, 419-426.	2.0	20
107	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.	3.3	19
108	Co-adsorption of CO molecules at the open ends of MgO nanotubes. Structural Chemistry, 2012, 23, 1981-1986.	2.0	19

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109	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.	3.3	19
110	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.	3.1	16
111	Theoretical study of cyano radical adsorption on (6,0) zigzag single-walled carbon nanotube. Monatshefte FÃ¼r Chemie, 2012, 143, 1463-1470.	1.8	16
112	DFT study of ozone dissociation on BC3 graphene with Stoneâ€“Wales defects. Journal of Molecular Modeling, 2014, 20, 2071.	1.8	16
113	Adsorption of nitrous oxide on the (6,0) magnesium oxide nanotube. Chinese Chemical Letters, 2012, 23, 1275-1278.	9.0	15
114	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.	3.3	15
115	Electronic, Energetic, and Geometric Properties of Methylene-Functionalized C60. Journal of Cluster Science, 2013, 24, 669-678.	3.3	14
116	The Alkali Metal Interactions with MgO Nanotubes. Bulletin of the Korean Chemical Society, 2012, 33, 1925-1928.	1.9	14
117	A Theoretical Study of OH and OCH3 Free Radical Adsorption on a Nanosized Tube of BC2N. Journal of Cluster Science, 2013, 24, 1011-1020.	3.3	12
118	A theoretical study on surface modification of a nanosized BC3 tube using C2H4 and its derivatives. Structural Chemistry, 2014, 25, 221-229.	2.0	12
119	Exohedral functionalization of C60 by [4+2] cycloaddition of multiple anthracenes. Structural Chemistry, 2014, 25, 785-791.	2.0	12
120	Adsorption of Na, Mg, and Al atoms on BN nanotubes. Thin Solid Films, 2012, 526, 139-142.	1.8	11
121	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.	1.8	11
122	Electric field effect on (6,0) zigzag single-walled aluminum nitride nanotube. Journal of Molecular Modeling, 2012, 18, 4477-4489.	1.8	10
123	Theoretical study on the functionalization of BC2N nanotube with amino groups. Journal of Molecular Modeling, 2013, 19, 2211-2216.	1.8	10
124	Application of hexaâ€periâ€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.	1.8	10
125	Adsorption and Electronic Structure Study of Imidazole on (6,0) Zigzag Single-Walled Boron Nitride Nanotube. Journal of Cluster Science, 2012, 24, 31.	3.3	9
126	The influence of Stone-Wales defects in nanographene on the performance of Na-ion batteries. Journal of Molecular Graphics and Modelling, 2020, 98, 107578.	2.4	9

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127	Covalent functionalization of AlN nanotubes with acetylene. Physica E: Low-Dimensional Systems and Nanostructures, 2013, 47, 147-151.	2.7	8
128	DFT study on [4+2] and [2+2] cycloadditions to [60] fullerene. Chemical Papers, 2014, 68, .	2.2	8
129	Electronic structure study of Si-doped (4,4) armchair single-walled boron phosphide nanotube as a semiconductor. Monatshefte FÃ¼r Chemie, 2012, 143, 1627-1635.	1.8	6
130	Adsorption of Thiophene on Aluminum Nitride Nanotubes. Phosphorus, Sulfur and Silicon and the Related Elements, 2013, 188, 1172-1177.	1.6	6
131	Density Functional Study of the Adsorption of Methanol and its Derivatives on Boron Nitride Nanotubes. Adsorption Science and Technology, 2013, 31, 767-776.	3.2	4
132	Explosive properties of nanosized diacetone diperoxide and its nitro derivatives: a DFT study. Monatshefte FÃ¼r Chemie, 2015, 146, 1401-1408.	1.8	3
133	Role of Diameter, Model, and Length of Boron Nitride Nanotubes in Adsorption of Formaldehyde. Fullerenes Nanotubes and Carbon Nanostructures, 2015, 23, 62-67.	2.1	2
134	NMR and NQR study of Si-doped (6,0) zigzag single-walled aluminum nitride nanotube as n or P â€“semiconductors. Journal of Molecular Modeling, 2012, 18, 4427-4436.	1.8	1
135	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.	1.6	1
136	Surface Modification of Carbon Nanotubes with Nitrenes: A DFT Study. Fullerenes Nanotubes and Carbon Nanostructures, 2015, 23, 326-331.	2.1	1