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	Au-decorated BN nanotube as a breathalyzer for potential medical applications. Journal of Molecular Liquids, 2020, 312, 113454.	4.9	30
2	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
3	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
4	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
5	Aluminum nitride nanotubes. Chemical Papers, 2017, 71, 881-893.	2.2	51
6	DFT studies of Hydrogen adsorption and dissociation on MgO nanotubes. Main Group Chemistry, 2016, 15, 107-116.	0.8	26
7	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
8	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
9	Sensing behavior of BN nanosheet toward nitrous oxide: A DFT study. Chinese Chemical Letters, 2015, 26, 1042-1045.	9.0	137
10	Explosive properties of nanosized diacetone diperoxide and its nitro derivatives: a DFT study. Monatshefte FÃ¼r Chemie, 2015, 146, 1401-1408.	1.8	3
11	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
12	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
13	Theoretical Study on the Al-Doped ZnO Nanoclusters for CO Chemical Sensors. Journal of Physical Chemistry C, 2015, 119, 6398-6404.	3.1	365
14	Adsorption of carbon monoxide on the pristine, B- and Al-doped C3N nanosheets. Journal of Molecular Modeling, 2015, 21, 116.	1.8	74
15	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
16	Theoretical study of carbonyl sulfide adsorption on Ag-doped SiC nanotubes. Journal of the Iranian Chemical Society, 2015, 12, 1071-1076.	2.2	76
17	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
18	First-principle study of methanol adsorption on Ni (Pd)-decorated graphene. Journal of the Iranian Chemical Society, 2015, 12, 751-756.	2.2	39

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19	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
20	Surface Modification of Carbon Nanotubes with Nitrenes: A DFT Study. Fullerenes Nanotubes and Carbon Nanostructures, 2015, 23, 326-331.	2.1	1
21	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
22	Adsorption of Formic Acid and Formate Anion on ZnO Nanocage: A DFT Study. Journal of Cluster Science, 2015, 26, 609-621.	3.3	43
23	Functionalization of the pristine and stone-wales defected BC3 graphenes with pyrene. Journal of Molecular Modeling, 2014, 20, 2539.	1.8	25
24	Hydrogen peroxide reduction in the oxygen vacancies of ZnO nanotubes. Thin Solid Films, 2014, 556, 566-570.	1.8	42
25	Influence of antisite defect upon decomposition of nitrous oxide over graphene-analogue SiC. Thin Solid Films, 2014, 552, 111-115.	1.8	28
26	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
27	Capture of carbon dioxide by a nanosized tube of BeO: a DFT study. Structural Chemistry, 2014, 25, 419-426.	2.0	20
28	DFT study on [4+2] and [2+2] cycloadditions to [60] fullerene. Chemical Papers, 2014, 68, .	2.2	8
29	Density-functional calculations of HCN adsorption on the pristine and Si-doped graphynes. Structural Chemistry, 2014, 25, 1-7.	2.0	79
30	Role of sodium decoration on the methane storage properties of BC3 nanosheet. Structural Chemistry, 2014, 25, 1083-1090.	2.0	36
31	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
32	Methanol-sensing characteristics of zinc oxide nanotubes: quantum chemical study. Monatshefte FÃ¼r Chemie, 2014, 145, 1253-1257.	1.8	40
33	DFT study of ozone dissociation on BC3 graphene with Stoneâ€“Wales defects. Journal of Molecular Modeling, 2014, 20, 2071.	1.8	16
34	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
35	Adsorption of H₂S at Stoneâ€“Wales defects of graphene-like BC₃: a computational study. Molecular Physics, 2014, 112, 2737-2745.	1.7	59
36	Ammonia borane reaction with a BN nanotube: a hydrogen storage route. Monatshefte FÃ¼r Chemie, 2014, 145, 1083-1087.	1.8	32

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37	The alkali and alkaline earth metal doped ZnO nanotubes: DFT studies. Physica B: Condensed Matter, 2014, 432, 105-110.	2.7	81
38	Exohedral functionalization of C60 by [4+2] cycloaddition of multiple anthracenes. Structural Chemistry, 2014, 25, 785-791.	2.0	12
39	Hydrogen fluoride on the pristine, Al and Si doped BC2N nanotubes: A computational study. Computational Materials Science, 2014, 82, 197-201.	3.0	27
40	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
41	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
42	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
43	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
44	ZnO Nanocluster as a Potential Catalyst for Dissociation of H2S Molecule. Journal of Cluster Science, 2013, 24, 341-347.	3.3	63
45	DFT study of NO2 adsorption on the AlN nanocones. Computational and Theoretical Chemistry, 2013, 1008, 20-26.	2.5	77
46	Tuning the electronic properties of C30B15N15 fullerene via encapsulation of alkali and alkali earth metals. Synthetic Metals, 2013, 177, 94-99.	3.9	37
47	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
48	Fluorination of BC3 nanotubes: DFT studies. Journal of Molecular Modeling, 2013, 19, 3941-3946.	1.8	23
49	Working Mechanism of a BC ₃ Nanotube Carbon Monoxide Gas Sensor. Communications in Theoretical Physics, 2013, 60, 113-118.	2.5	24
50	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
51	Transition metal atom adsorptions on a boron nitride nanocage. Structural Chemistry, 2013, 24, 1039-1044.	2.0	33
52	Carbon nanocone as an ammonia sensor: DFT studies. Structural Chemistry, 2013, 24, 1099-1103.	2.0	71
53	Formaldehyde adsorption on the interior and exterior surfaces of CN nanotubes. Structural Chemistry, 2013, 24, 1331-1337.	2.0	36
54	Ab initio study of NH3 and H2O adsorption on pristine and Na-doped MgO nanotubes. Structural Chemistry, 2013, 24, 165-170.	2.0	80

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55	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
56	A DFT study on the sensing behavior of a BC2N nanotube toward formaldehyde. Journal of Molecular Modeling, 2013, 19, 3843-3850.	1.8	63
57	Sensing behavior of Al-rich AlN nanotube toward hydrogen cyanide. Journal of Molecular Modeling, 2013, 19, 2197-2203.	1.8	63
58	Electronic, energetic, and structural properties of C- and Si-doped Mg12O12 nano-cages. Computational Materials Science, 2013, 79, 352-355.	3.0	30
59	DFT study of the dissociative adsorption of HF on an AlN nanotube. Comptes Rendus Chimie, 2013, 16, 985-989.	0.5	58
60	DFT study on the functionalization of a BN nanotube with sulfamide. Applied Surface Science, 2013, 266, 182-187.	6.1	87
61	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
62	Response of Si- and Al-doped graphenes toward HCN: A computational study. Applied Surface Science, 2013, 265, 412-417.	6.1	151
63	Electronic response of BC3 nanotube to CS2 molecules: DFT studies. Computational and Theoretical Chemistry, 2013, 1008, 1-7.	2.5	23
64	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
65	Hydrogen dissociation on diene-functionalized carbon nanotubes. Journal of Molecular Modeling, 2013, 19, 255-261.	1.8	72
66	Carbon nanotube functionalization with carboxylic derivatives: a DFT study. Journal of Molecular Modeling, 2013, 19, 391-396.	1.8	63
67	Adsorption of CO molecule on AlN nanotubes by parallel electric field. Journal of Molecular Modeling, 2013, 19, 859-870.	1.8	32
68	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
69	Nitrous oxide adsorption on pristine and Si-doped AlN nanotubes. Journal of Molecular Modeling, 2013, 19, 943-949.	1.8	36
70	Covalent functionalization of AlN nanotubes with acetylene. Physica E: Low-Dimensional Systems and Nanostructures, 2013, 47, 147-151.	2.7	8
71	Selective adsorption behavior of BC2N nanotubes toward fluoride and chloride. Solid State Communications, 2013, 159, 8-12.	1.9	24
72	Sensing behavior of Al and Si doped BC3 graphenes to formaldehyde. Sensors and Actuators B: Chemical, 2013, 181, 829-834.	7.8	188

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73	Decomposition of methanol on nanosized tube of magnesium oxide: A theoretical study. Computational Materials Science, 2013, 79, 182-186.	3.0	32
74	Ammonia monitoring by carbon nitride nanotubes: A density functional study. Thin Solid Films, 2013, 534, 650-654.	1.8	75
75	A density functional theory study on acetylene-functionalized BN nanotubes. Structural Chemistry, 2013, 24, 1007-1013.	2.0	28
76	Structural and electronic properties of pyrrolidine-functionalized [60]fullerenes. Journal of Physics and Chemistry of Solids, 2013, 74, 1594-1598.	4.0	70
77	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
78	Electronic, Energetic, and Geometric Properties of Methylene-Functionalized C60. Journal of Cluster Science, 2013, 24, 669-678.	3.3	14
79	Exohedral and endohedral adsorption of alkaline earth cations in BN nanocluster. Journal of Molecular Modeling, 2013, 19, 1445-1450.	1.8	33
80	Theoretical study on the functionalization of BC2N nanotube with amino groups. Journal of Molecular Modeling, 2013, 19, 2211-2216.	1.8	10
81	NH3 on a BC3 nanotube: effect of doping and decoration of aluminum. Journal of Molecular Modeling, 2013, 19, 3793-3798.	1.8	20
82	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
83	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
84	Quantum chemical analysis on hydrogenated Zn12O12 nanoclusters. Comptes Rendus Chimie, 2013, 16, 122-128.	0.5	21
85	Al-doped graphene-like BN nanosheet as a sensor for para-nitrophenol: DFT study. Superlattices and Microstructures, 2013, 59, 115-122.	3.1	185
86	Carbon nitride nanotube as a sensor for alkali and alkaline earth cations. Applied Surface Science, 2013, 264, 699-706.	6.1	82
87	Fluorination of the exterior surface of AlN nanotube: A DFT study. Superlattices and Microstructures, 2013, 53, 9-15.	3.1	22
88	NO2 detection by nanosized AlN sheet in the presence of NH3: DFT studies. Applied Surface Science, 2013, 274, 217-220.	6.1	117
89	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
90	Adsorption of Thiophene on Aluminum Nitride Nanotubes. Phosphorus, Sulfur and Silicon and the Related Elements, 2013, 188, 1172-1177.	1.6	6

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91	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
92	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
93	B12N12 Nano-cage as Potential Sensor for NO2 Detection. Chinese Journal of Chemical Physics, 2012, 25, 60-64.	1.3	126
94	First Principles Study on Encapsulation of Alkali Metals into ZnO Nanocage. Chinese Journal of Chemical Physics, 2012, 25, 671-675.	1.3	23
95	Nitrate adsorption by carbon nanotubes in the vacuum and aqueous phase. Monatshefte FÃ¼r Chemie, 2012, 143, 1623-1626.	1.8	68
96	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
97	Cation-Ï€ interaction of alkali metal ions with C24 fullerene: a DFT study. Journal of Molecular Modeling, 2012, 18, 3535-3540.	1.8	81
98	Electric field effect on (6,0) zigzag single-walled aluminum nitride nanotube. Journal of Molecular Modeling, 2012, 18, 4477-4489.	1.8	10
99	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
100	Electronic sensor for sulfide dioxide based on AlN nanotubes: a computational study. Journal of Molecular Modeling, 2012, 18, 4745-4750.	1.8	80
101	Adsorption of nitrous oxide on the (6,0) magnesium oxide nanotube. Chinese Chemical Letters, 2012, 23, 1275-1278.	9.0	15
102	Can aluminum nitride nanotubes detect the toxic NH3 molecules?. Physica E: Low-Dimensional Systems and Nanostructures, 2012, 44, 1357-1360.	2.7	85
103	Energetic, structural, and electronic properties of hydrogenated Al12P12 nanocluster. Physica E: Low-Dimensional Systems and Nanostructures, 2012, 44, 1436-1440.	2.7	37
104	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
105	Theoretical study of CO adsorption on the surface of BN, AlN, BP and AlP nanotubes. Surface Science, 2012, 606, 981-985.	1.9	152
106	Adsorption and dissociation of Cl2 molecule on ZnO nanocluster. Applied Surface Science, 2012, 258, 8171-8176.	6.1	117
107	Functionalization of [60] fullerene with butadienes: A DFT study. Applied Surface Science, 2012, 258, 8980-8984.	6.1	59
108	Quantum chemical study of fluorinated AlN nano-cage. Applied Surface Science, 2012, 259, 631-636.	6.1	97

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109	Selective function of Al12N12 nano-cage towards NO and CO molecules. Computational Materials Science, 2012, 62, 71-74.	3.0	136
110	Theoretical investigation of C60 fullerene functionalization with tetrazine. Computational and Theoretical Chemistry, 2012, 992, 164-167.	2.5	73
111	A computational study of AlN nanotube as an oxygen detector. Chinese Chemical Letters, 2012, 23, 965-968.	9.0	76
112	Theoretical study of hydrogen adsorption on the B12P12 fullerene-like nanocluster. Computational Materials Science, 2012, 54, 115-118.	3.0	95
113	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
114	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
115	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
116	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
117	Adsorption of Na, Mg, and Al atoms on BN nanotubes. Thin Solid Films, 2012, 526, 139-142.	1.8	11
118	Detection of phosgene by Sc-doped BN nanotubes: A DFT study. Sensors and Actuators B: Chemical, 2012, 171-172, 846-852.	7.8	292
119	Theoretical study of cyano radical adsorption on (6,0) zigzag single-walled carbon nanotube. Monatshefte FÃ¼r Chemie, 2012, 143, 1463-1470.	1.8	16
120	Interaction of small molecules (NO, H2, N2, and CH4) with BN nanocluster surface. Structural Chemistry, 2012, 23, 1567-1572.	2.0	103
121	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
122	Co-adsorption of CO molecules at the open ends of MgO nanotubes. Structural Chemistry, 2012, 23, 1981-1986.	2.0	19
123	A theoretical study of CO adsorption on aluminum nitride nanotubes. Structural Chemistry, 2012, 23, 653-657.	2.0	77
124	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
125	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
126	A comparative study on the B12N12, Al12N12, B12P12 and Al12P12 fullerene-like cages. Journal of Molecular Modeling, 2012, 18, 2653-2658.	1.8	160

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127	Theoretical study of aluminum nitride nanotubes for chemical sensing of formaldehyde. Sensors and Actuators B: Chemical, 2012, 161, 1025-1029.	7.8	248
128	AlN nanotube as a potential electronic sensor for nitrogen dioxide. Microelectronics Journal, 2012, 43, 452-455.	2.0	96
129	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
130	A DFT Study on CO₂Interaction with a BN Nano-Cage. Bulletin of the Korean Chemical Society, 2012, 33, 3338-3342.	1.9	31
131	The Alkali Metal Interactions with MgO Nanotubes. Bulletin of the Korean Chemical Society, 2012, 33, 1925-1928.	1.9	14
132	Toxic CO detection by B12N12 nanocluster. Microelectronics Journal, 2011, 42, 1400-1403.	2.0	124
133	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
134	Chemisorption of NH3 at the open ends of boron nitride nanotubes: a DFT study. Structural Chemistry, 2011, 22, 183-188.	2.0	88
135	The effect of surface curvature of aluminum nitride nanotubes on the adsorption of NH3. Structural Chemistry, 2011, 22, 1261-1265.	2.0	72
136	Interaction of NH3 with aluminum nitride nanotube: Electrostatic vs. covalent. Physica E: Low-Dimensional Systems and Nanostructures, 2011, 43, 1717-1719.	2.7	84