Zargham Bagheri

List of Publications by Year
in descending order

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Version: 2024-02-01

47 papers	3,430 citations	126907 33 h-index	214800 47 g-index
47 all docs	47 docs citations	47 times ranked	1280 citing authors

#	Article	IF	Citations
1	Detection of phosgene by Sc-doped BN nanotubes: A DFT study. Sensors and Actuators B: Chemical, 2012, 171-172, 846-852.	7.8	292
2	Theoretical study of aluminum nitride nanotubes for chemical sensing of formaldehyde. Sensors and Actuators B: Chemical, 2012, 161, 1025-1029.	7.8	248
3	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
4	A comparative study on the B12N12, Al12N12, B12P12 and Al12P12 fullerene-like cages. Journal of Molecular Modeling, 2012, 18, 2653-2658.	1.8	160
5	Selective function of Al12N12 nano-cage towards NO and CO molecules. Computational Materials Science, 2012, 62, 71-74.	3.0	136
6	B12N12 Nano-cage as Potential Sensor for NO2 Detection. Chinese Journal of Chemical Physics, 2012, 25, 60-64.	1.3	126
7	Adsorption and dissociation of Cl2 molecule on ZnO nanocluster. Applied Surface Science, 2012, 258, 8171-8176.	6.1	117
8	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
9	Interaction of small molecules (NO, H2, N2, and CH4) with BN nanocluster surface. Structural Chemistry, 2012, 23, 1567-1572.	2.0	103
10	B 24 N 24 fullerene as a carrier for 5-fluorouracil anti-cancer drug delivery: DFT studies. Journal of Molecular Graphics and Modelling, 2017, 77, 17-24.	2.4	103
11	Quantum chemical study of fluorinated AlN nano-cage. Applied Surface Science, 2012, 259, 631-636.	6.1	97
12	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
13	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
14	Cation-Ï€ interaction of alkali metal ions with C24 fullerene: a DFT study. Journal of Molecular Modeling, 2012, 18, 3535-3540.	1.8	81
15	Electronic sensor for sulfide dioxide based on AlN nanotubes: a computational study. Journal of Molecular Modeling, 2012, 18, 4745-4750.	1.8	80
16	Ab initio study of NH3 and H2O adsorption on pristine and Na-doped MgO nanotubes. Structural Chemistry, 2013, 24, 165-170.	2.0	80
17	Density-functional calculations of HCN adsorption on the pristine and Si-doped graphynes. Structural Chemistry, 2014, 25, 1-7.	2.0	79
18	A theoretical study of CO adsorption on aluminum nitride nanotubes. Structural Chemistry, 2012, 23, 653-657.	2.0	77

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19	DFT study of NO2 adsorption on the AlN nanocones. Computational and Theoretical Chemistry, 2013, 1008, 20-26.	2.5	77
20	Theoretical study of carbonyl sulfide adsorption on Ag-doped SiC nanotubes. Journal of the Iranian Chemical Society, 2015, 12, 1071-1076.	2.2	76
21	Theoretical investigation of C60 fullerene functionalization with tetrazine. Computational and Theoretical Chemistry, 2012, 992, 164-167.	2.5	73
22	Hydrogen dissociation on diene-functionalized carbon nanotubes. Journal of Molecular Modeling, 2013, 19, 255-261.	1.8	72
23	Carbon nanocone as an ammonia sensor: DFT studies. Structural Chemistry, 2013, 24, 1099-1103.	2.0	71
24	Nitrate adsorption by carbon nanotubes in the vacuum and aqueous phase. Monatshefte FÃ¼r Chemie, 2012, 143, 1623-1626.	1.8	68
25	Carbon nanotube functionalization with carboxylic derivatives: a DFT study. Journal of Molecular Modeling, 2013, 19, 391-396.	1.8	63
26	Functionalization of [60] fullerene with butadienes: A DFT study. Applied Surface Science, 2012, 258, 8980-8984.	6.1	59
27	Application of C 30 B 15 N 15 heterofullerene in the isoniazid drug delivery: DFT studies. Physica E: Low-Dimensional Systems and Nanostructures, 2017, 89, 72-76.	2.7	41
28	On the utility of C24 fullerene framework for Li-ion batteries: Quantum chemical analysis. Applied Surface Science, 2016, 383, 294-299.	6.1	38
29	Tuning the electronic properties of C30B15N15 fullerene via encapsulation of alkali and alkali earth metals. Synthetic Metals, 2013, 177, 94-99.	3.9	37
30	Formaldehyde adsorption on the interior and exterior surfaces of CN nanotubes. Structural Chemistry, 2013, 24, 1331-1337.	2.0	36
31	Nitrous oxide adsorption on pristine and Si-doped AlN nanotubes. Journal of Molecular Modeling, 2013, 19, 943-949.	1.8	36
32	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
33	Transition metal atom adsorptions on a boron nitride nanocage. Structural Chemistry, 2013, 24, 1039-1044.	2.0	33
34	Exohedral and endohedral adsorption of alkaline earth cations in BN nanocluster. Journal of Molecular Modeling, 2013, 19, 1445-1450.	1.8	33
35	Li interactions with the B 40 fullerene and its application in Li-ion batteries: DFT studies. Physica E: Low-Dimensional Systems and Nanostructures, 2017, 89, 148-154.	2.7	33
36	Adsorption and dissociation of nitrous oxide on pristine and defective BeO and ZnO nanotubes: DFT studies. Monatshefte FÃ¼r Chemie, 2014, 145, 1745-1752.	1.8	32

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37	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
38	A density functional theory study on acetylene-functionalized BN nanotubes. Structural Chemistry, 2013, 24, 1007-1013.	2.0	28
39	Physisorption to chemisorption transition of H2S on carbon nanocone induced by decoration of Be2O2 cluster. Journal of the Iranian Chemical Society, 2015, 12, 1099-1106.	2.2	26
40	Functionalization of the pristine and stone-wales defected BC3 graphenes with pyrene. Journal of Molecular Modeling, 2014, 20, 2539.	1.8	25
41	First Principles Study on Encapsulation of Alkali Metals into ZnO Nanocage. Chinese Journal of Chemical Physics, 2012, 25, 671-675.	1.3	23
42	Electronic response of BC3 nanotube to CS2 molecules: DFT studies. Computational and Theoretical Chemistry, 2013, 1008, 1-7.	2.5	23
43	Co-adsorption of CO molecules at the open ends of MgO nanotubes. Structural Chemistry, 2012, 23, 1981-1986.	2.0	19
44	Adsorption and dissociation of hydrogen peroxide on the defected carbon nanotubes. Structural Chemistry, 2015, 26, 485-490.	2.0	18
45	Electronic, Energetic, and Geometric Properties of Methylene-Functionalized C60. Journal of Cluster Science, 2013, 24, 669-678.	3.3	14
46	DFT study on the adsorption and dissociation of hydrogen sulfide on MgO nanotube. Structural Chemistry, 2014, 25, 495-501.	2.0	13
47	DFT study on the chemical sensitivity of C3N nanotubes toward acetone. Physica E: Low-Dimensional Systems and Nanostructures, 2016, 76, 151-157.	2.7	8