Javad Beheshtian

List of Publications by Citations

98 papers	4,237 citations	40 h-index	63 g-index
103 ext. papers	4,687 ext. citations	3.5 avg, IF	5.95 L-index

#	Paper	IF	Citations
98	Detection of phosgene by Sc-doped BN nanotubes: A DFT study. *Sensors and Actuators B: Chemical*, **2012**, 171-172, 846-852	8.5	240
97	Sensing behavior of Al and Si doped BC3 graphenes to formaldehyde. *Sensors and Actuators B: Chemical*, **2013**, 181, 829-834	8.5	158
96	A comparative study on the B12N12, Al12N12, B12P12 and Al12P12 fullerene-like cages. *Journal of Molecular Modeling*, **2012**, 18, 2653-8	2	129
95	Microporous titania–silica nanocomposite catalyst-adsorbent for ultra-deep oxidative desulfurization. *Applied Catalysis B: Environmental*, **2016**, 180, 65-77	21.8	128
94	Theoretical study of CO adsorption on the surface of BN, AlN, BP and AlP nanotubes. *Surface Science*, **2012**, 606, 981-985	1.8	125
93	Selective function of Al12N12 nano-cage towards NO and CO molecules. *Computational Materials Science*, **2012**, 62, 71-74	3.2	113
92	Highly active Fe2O3-doped TiO2 photocatalyst for degradation of trichloroethylene in air under UV and visible light irradiation: Experimental and computational studies. *Applied Catalysis B: Environmental*, **2015**, 165, 209-221	21.8	103
91	Toxic CO detection by B12N12 nanocluster. *Microelectronics Journal*, **2011**, 42, 1400-1403	1.8	103
90	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
89	B12N12 Nano-cage as Potential Sensor for NO2 Detection. *Chinese Journal of Chemical Physics*, **2012**, 25, 60-64	0.9	100
88	Adsorption and dissociation of Cl2 molecule on ZnO nanocluster. *Applied Surface Science*, **2012**, 258, 8171-8176	6.7	95
87	Van der Waals pressure and its effect on trapped interlayer molecules. *Nature Communications*, **2016**, 7, 12168	17.4	91
86	Computational study of CO and NO adsorption on magnesium oxide nanotubes. *Physica E: Low-Dimensional Systems and Nanostructures*, **2011**, 44, 546-549	3	88
85	Quantum chemical study of fluorinated AlN nano-cage. *Applied Surface Science*, **2012**, 259, 631-636	6.7	86
84	Interaction of small molecules (NO, H2, N2, and CH4) with BN nanocluster surface. *Structural Chemistry*, **2012**, 23, 1567-1572	1.8	86
83	AlN nanotube as a potential electronic sensor for nitrogen dioxide. *Microelectronics Journal*, **2012**, 43, 452-455	1.8	84
82	Chemisorption of NH3 at the open ends of boron nitride nanotubes: a DFT study. *Structural Chemistry*, **2011**, 22, 183-188	1.8	84

81	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
80	Theoretical study of hydrogen adsorption on the B12P12 fullerene-like nanocluster. *Computational Materials Science*, **2012**, 54, 115-118	3.2	83
79	The H2 dissociation on the BN, AlN, BP and AlP nanotubes: a comparative study. *Journal of Molecular Modeling*, **2012**, 18, 2343-8	2	80
78	Carbon nitride nanotube as a sensor for alkali and alkaline earth cations. *Applied Surface Science*, **2013**, 264, 699-706	6.7	80
77	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
76	DFT study on the functionalization of a BN nanotube with sulfamide. *Applied Surface Science*, **2013**, 266, 182-187	6.7	78
75	Ab initio study of NH3 and H2O adsorption on pristine and Na-doped MgO nanotubes. *Structural Chemistry*, **2013**, 24, 165-170	1.8	76
74	Interaction of NH3 with aluminum nitride nanotube: Electrostatic vs. covalent. *Physica E: Low-Dimensional Systems and Nanostructures*, **2011**, 43, 1717-1719	3	76
73	A theoretical study of CO adsorption on aluminum nitride nanotubes. *Structural Chemistry*, **2012**, 23, 653-657	1.8	74
72	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
71	Electronic sensor for sulfide dioxide based on AlN nanotubes: a computational study. *Journal of Molecular Modeling*, **2012**, 18, 4745-50	2	70
70	Experimental and Theoretical Study of Enhanced Photocatalytic Activity of Mg-Doped ZnO NPs and ZnO/rGO Nanocomposites. *Chemistry - an Asian Journal*, **2018**, 13, 194-203	4.5	67
69	Nitrate adsorption by carbon nanotubes in the vacuum and aqueous phase. *Monatshefte F□ Chemie* , **2012**, 143, 1623-1626	1.4	65
68	Hydrogen dissociation on diene-functionalized carbon nanotubes. *Journal of Molecular Modeling*, **2013**, 19, 255-61	2	63
67	The effect of surface curvature of aluminum nitride nanotubes on the adsorption of NH3. *Structural Chemistry*, **2011**, 22, 1261-1265	1.8	63
66	Density-functional calculations of HCN adsorption on the pristine and Si-doped graphynes. *Structural Chemistry*, **2014**, 25, 1-7	1.8	62
65	Ammonia monitoring by carbon nitride nanotubes: A density functional study. *Thin Solid Films*, **2013** , 534, 650-654	2.2	62
64	Theoretical investigation of C60 fullerene functionalization with tetrazine. *Computational and Theoretical Chemistry*, **2012**, 992, 164-167	2	61

63	Sensing behavior of Al-rich AlN nanotube toward hydrogen cyanide. *Journal of Molecular Modeling*, **2013**, 19, 2197-203	2	58
62	Carbon nanotube functionalization with carboxylic derivatives: a DFT study. *Journal of Molecular Modeling*, **2013**, 19, 391-6	2	58
61	Highly sensitive and selective ethanol and acetone gas sensors by adding some dopants (Mn, Fe, Co, Ni) onto hexagonal ZnO plates. *RSC Advances*, **2016**, 6, 7838-7845	3.7	57
60	Functionalization of [60] fullerene with butadienes: A DFT study. *Applied Surface Science*, **2012**, 258, 8980-8984	6.7	55
59	Theoretical prediction of silicene as a new candidate for the anode of lithium-ion batteries. *Physical Chemistry Chemical Physics*, **2015**, 17, 29689-96	3.6	48
58	Boron Nitride Monolayer: A Strain-Tunable Nanosensor. *Journal of Physical Chemistry C*, **2013**, 117, 13261-13267	4.8	37
57	Induced polarization and electronic properties of carbon-doped boron nitride nanoribbons. *Physical Review B*, **2012**, 86,	3.3	36
56	Computational study on the characteristics of the interaction in linear urea clusters. *International Journal of Quantum Chemistry*, **2011**, 111, 3184-3195	2.1	36
55	Formaldehyde adsorption on the interior and exterior surfaces of CN nanotubes. *Structural Chemistry*, **2013**, 24, 1331-1337	1.8	33
54	A computational study of water adsorption on boron nitride nanotube. *Structural Chemistry*, **2010**, 21, 903-908	1.8	33
53	DFT study of NH3 adsorption on the (5,0), (8,0), (5,5) and (6,6) single-walled carbon nanotubes. Calculated binding energies, NMR and NQR parameters. *Physica B: Condensed Matter*, **2010**, 405, 1455-1460	2.8	32
52	Theoretical 14N nuclear quadrupole resonance parameters for sulfa drugs: sulfamerazine and sulfathiazole. *Journal of Molecular Graphics and Modelling*, **2008**, 27, 326-31	2.8	29
51	Hydrogen storage by BeO nano-cage: A DFT study. *Applied Surface Science*, **2016**, 368, 76-81	6.7	28
50	Exohedral and endohedral adsorption of alkaline earth cations in BN nanocluster. *Journal of Molecular Modeling*, **2013**, 19, 1445-50	2	27
49	Arsenic interactions with a fullerene-like BN cage in the vacuum and aqueous phase. *Journal of Molecular Modeling*, **2013**, 19, 833-7	2	26
48	Nitrous oxide adsorption on pristine and Si-doped AlN nanotubes. *Journal of Molecular Modeling*, **2013**, 19, 943-9	2	26
47	Preparation of uniform 2D ZnO nanostructures by the ionic liquid-assisted sonochemical method and their optical properties. *Ceramics International*, **2014**, 40, 7769-7774	5.1	25
46	Electrochemical and DFT study of an anticancer and active anthelmintic drug at carbon nanostructured modified electrode. *Materials Science and Engineering C*, **2016**, 69, 1345-53	8.3	23

45	Preparation of Cu2O nanostructures by changing reducing agent and their optical properties. *Materials Letters*, **2015**, 153, 1-4	3.3	22
44	Reversible structural transition in nanoconfined ice. *Physical Review B*, **2017**, 95,	3.3	21
43	Natural pigments in dye-sensitized solar cell (DSSC): a DFT-TDDFT study. *Journal of the Iranian Chemical Society*, **2019**, 16, 795-805	2	21
42	Co-adsorption of CO molecules at the open ends of MgO nanotubes. *Structural Chemistry*, **2012**, 23, 1981-1986	1.8	18
41	Spiral graphone and one-sided fluorographene nanoribbons. *Physical Review B*, **2013**, 87,	3.3	17
40	Electronic and optical properties of vacancy and B, N, O and F doped graphene: DFT study. *Opto-electronics Review*, **2019**, 27, 130-136	2.4	16
39	Graphene-silicene bilayer: A nanocapacitor with permanent dipole and piezoelectricity effect. *Physical Review B*, **2015**, 92,	3.3	16
38	Effects of functionalization and side defects on single-photon emission in boron nitride quantum dots. *Physical Review B*, **2017**, 96,	3.3	15
37	First-Principles Study of Water Nanotubes Captured Inside Carbon/Boron Nitride Nanotubes. *Langmuir*, **2018**, 34, 11176-11187	4	14
36	The Alkali Metal Interactions with MgO Nanotubes. *Bulletin of the Korean Chemical Society*, **2012**, 33, 1925-1928	1.2	14
35	Ultrasonic route synthesis, characterization and electrochemical study of graphene oxide and reduced graphene oxide. *Research on Chemical Intermediates*, **2019**, 45, 487-505	2.8	13
34	Phase transition and mechanical properties of cesium bismuth silver halide double perovskites (CsAgBiX, X = Cl, Br, I): a DFT approach. *Physical Chemistry Chemical Physics*, **2020**, 22, 5959-5968	3.6	12
33	Selective separation behavior of graphene flakes in interaction with halide anions in the presence of an external electric field. *Physical Chemistry Chemical Physics*, **2016**, 18, 7293-9	3.6	12
32	Experimental and theoretical study of CO adsorption on the surface of single phase hexagonally plate ZnO. *Applied Surface Science*, **2014**, 315, 8-15	6.7	12
31	Doping effect on the adsorption of NH3 molecule onto graphene quantum dot: From the physisorption to the chemisorption. *Journal of Applied Physics*, **2013**, 114, 124307	2.5	12
30	Computational study of ammonia adsorption on the perfect and rippled graphene sheet. *Physica B: Condensed Matter*, **2013**, 429, 52-56	2.8	11
29	Adsorption of Na, Mg, and Al atoms on BN nanotubes. *Thin Solid Films*, **2012**, 526, 139-142	2.2	11
28	DFT study of NH3(H2O)n=0,1,2,3 complex adsorption on the (8, 0) single-walled carbon nanotube. *Computational Materials Science*, **2010**, 48, 655-657	3.2	11

27	Theoretical study on the functionalization of BCN nanotube with amino groups. *Journal of Molecular Modeling*, **2013**, 19, 2211-6	2	10
26	Electro-Optical Properties of Monolayer and Bilayer Pentagonal BN: First Principles Study. *Nanomaterials*, **2020**, 10,	5.4	8
25	Synthesis of undoped and Fe nanoparticles doped SnO2 nanostructure: study of structural, optical and electrocatalytic properties. *Journal of Materials Science: Materials in Electronics*, **2017**, 28, 7568-7574	2.1	7
24	A density functional study of 15N chemical shielding tensors in quinolines. *Chemical Physics Letters*, **2009**, 476, 196-200	2.5	7
23	Photo-oxidation of phenylazonaphthol dyes and their reactivity analysis in the gas phase and adsorbed on cellulose fibers states using DFT and TD-DFT. *Dyes and Pigments*, **2011**, 89, 16-22	4.6	7
22	Voltammetric Sensor Based on Fe-doped ZnO and TiO2 Nanostructures-modified Carbon-paste Electrode for Determination of Levodopa. *Journal of Electronic Materials*, **2017**, 46, 5657-5663	1.9	6
21	Toxic CO detection by Li-encapsulated fullerene-like BeO. *Structural Chemistry*, **2018**, 29, 231-241	1.8	6
20	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
19	Effect of nitrogen doping on electronic and optical properties of ZnO sheet: DFT+U study. *Computational Condensed Matter*, **2018**, 15, 1-6	1.7	5
18	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
17	Synthesis, identification, crystal structure and theoretical study of a Ce(IV) complex. *Journal of the Iranian Chemical Society*, **2014**, 11, 1353-1361	2	3
16	The electronic and optical properties of 3d transition metals doped silicene sheet: A DFT study. *Materials Research Express*, **2019**, 6, 126326	1.7	3
15	Electronic, magnetic and optical properties of Fe-doped nano-BN sheet: DFT study. *Indian Journal of Physics*, **2021**, 95, 823-831	1.4	3
14	Helium selectivity of H-, B-, N-, and F- doped nanoporous graphene membranes in the presence of natural gas: A density functional theory study. *Superlattices and Microstructures*, **2020**, 141, 106478	2.8	2
13	15N CHEMICAL SHIFT CALCULATIONS AND NATURAL BONDING ORBITAL ANALYSES OF (BENZAMIDE)n = 1 - 6 CLUSTERS. *Journal of Theoretical and Computational Chemistry*, **2009**, 08, 973-982	1.8	2
12	Hydrogenated graphene as an ultraviolet optomechanical sensor.. *RSC Advances*, **2020**, 10, 26197-26211	3.7	2
11	A DFT study on the potential application of pristine, B and N doped carbon nanocones in potassium-ion batteries. *Journal of Molecular Modeling*, **2021**, 27, 168	2	2
10	A computational study on the novel defects of graphene quantum dot as a promising anode material for sodium ion battery. *Materials Chemistry and Physics*, **2021**, 265, 124484	4.4	2

9	Boron nitride nanochannels encapsulating a water/heavy water layer for energy applications.. *RSC Advances*, **2019**, 9, 5901-5907	3.7	2
8	Nanoscale investigation of the influence of water on the elastic properties of C-S-H gel by molecular simulation. *Proceedings of the Institution of Mechanical Engineers, Part L: Journal of Materials: Design and Applications*, **2019**, 233, 1295-1306	1.3	2
7	Ab Initio Study of Mono-Layer Graphene as an Electronical or Optical Sensor for Detecting B, N, O and F Atoms. *Journal of Electronic Materials*, **2019**, 48, 4265-4272	1.9	1
6	Interfacial properties of water/heavy water layer encapsulate in bilayer graphene nanochannel and nanocapacitor. *Journal of Materials Science: Materials in Electronics*, **2019**, 30, 11964-11975	2.1	1
5	Theoretical investigation of azo dyes adsorbed on cellulose fibers: 1. Electronic and bonding structures. *Journal of the Iranian Chemical Society*, **2013**, 10, 985-999	2	1
4	Theoretical investigation of azo dyes adsorbed on cellulose fibers: 2. Spectroscopic study. *Journal of the Iranian Chemical Society*, **2014**, 11, 111-121	2	1
3	A computational study on the BN and AlN nanocones as anode materials for K-ion batteries. *Applied Surface Science*, **2021**, 544, 148793	6.7	1
2	Electrodeposition of CoxNiVyOz Ternary Nanopetals on Bare and rGO-Coated Nickel Foam for High-Performance Supercapacitor Application. *Nanomaterials*, **2022**, 12, 1894	5.4	1
1	Experimental and Theoretical Study of Porous Al2O3. *Transactions of the Indian Institute of Metals*, **2021**, 74, 381-386	1.2	