Javad Beheshtian

List of Publications by Year
in descending order

102	5,131	71102	88630
papers	citations	41 h-index	70 g-index

103	103	103	3294
all docs	docs citations	times ranked	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	Sensing behavior of Al and Si doped BC3 graphenes to formaldehyde. Sensors and Actuators B: Chemical, 2013, 181, 829-834.	7.8	188
3	A comparative study on the B12N12, Al12N12, B12P12 and Al12P12 fullerene-like cages. Journal of Molecular Modeling, 2012, 18, 2653-2658.	1.8	160
4	Microporous titaniaâ€“silica nanocomposite catalyst-adsorbent for ultra-deep oxidative desulfurization. Applied Catalysis B: Environmental, 2016, 180, 65-77.	20.2	153
5	Theoretical study of CO adsorption on the surface of BN, AlN, BP and AlP nanotubes. Surface Science, 2012, 606, 981-985.	1.9	152
6	Van der Waals pressure and its effect on trapped interlayer molecules. Nature Communications, 2016, 7, 12168.	12.8	137
7	Selective function of Al12N12 nano-cage towards NO and CO molecules. Computational Materials Science, 2012, 62, 71-74.	3.0	136
8	A DFT study on the functionalization of a BN nanosheet with PCX, (PC=phenyl carbamate, X=OCH3, CH3,) Tj ETQq0 0 0 rgBT /Overlock	6.1	136
9	B12N12 Nano-cage as Potential Sensor for NO2 Detection. Chinese Journal of Chemical Physics, 2012, 25, 60-64.	1.3	126
10	Toxic CO detection by B12N12 nanocluster. Microelectronics Journal, 2011, 42, 1400-1403.	2.0	124
11	Adsorption and dissociation of Cl2 molecule on ZnO nanocluster. Applied Surface Science, 2012, 258, 8171-8176.	6.1	117
12	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.	20.2	117
13	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
14	Interaction of small molecules (NO, H2, N2, and CH4) with BN nanocluster surface. Structural Chemistry, 2012, 23, 1567-1572.	2.0	103
15	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
16	Quantum chemical study of fluorinated AlN nano-cage. Applied Surface Science, 2012, 259, 631-636.	6.1	97
17	AlN nanotube as a potential electronic sensor for nitrogen dioxide. Microelectronics Journal, 2012, 43, 452-455.	2.0	96
18	Theoretical study of hydrogen adsorption on the B12P12 fullerene-like nanocluster. Computational Materials Science, 2012, 54, 115-118.	3.0	95

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19	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
20	Chemisorption of NH3 at the open ends of boron nitride nanotubes: a DFT study. Structural Chemistry, 2011, 22, 183-188.	2.0	88
21	DFT study on the functionalization of a BN nanotube with sulfamide. Applied Surface Science, 2013, 266, 182-187.	6.1	87
22	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
23	Interaction of NH3 with aluminum nitride nanotube: Electrostatic vs. covalent. Physica E: Low-Dimensional Systems and Nanostructures, 2011, 43, 1717-1719.	2.7	84
24	Experimental and Theoretical Study of Enhanced Photocatalytic Activity of Mgâ€Doped ZnO NPs and ZnO/rGO Nanocomposites. Chemistry - an Asian Journal, 2018, 13, 194-203.	3.3	83
25	Carbon nitride nanotube as a sensor for alkali and alkaline earth cations. Applied Surface Science, 2013, 264, 699-706.	6.1	82
26	Electronic sensor for sulfide dioxide based on AlN nanotubes: a computational study. Journal of Molecular Modeling, 2012, 18, 4745-4750.	1.8	80
27	Ab initio study of NH3 and H2O adsorption on pristine and Na-doped MgO nanotubes. Structural Chemistry, 2013, 24, 165-170.	2.0	80
28	Density-functional calculations of HCN adsorption on the pristine and Si-doped graphynes. Structural Chemistry, 2014, 25, 1-7.	2.0	79
29	A theoretical study of CO adsorption on aluminum nitride nanotubes. Structural Chemistry, 2012, 23, 653-657.	2.0	77
30	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
31	Ammonia monitoring by carbon nitride nanotubes: A density functional study. Thin Solid Films, 2013, 534, 650-654.	1.8	75
32	Theoretical investigation of C60 fullerene functionalization with tetrazine. Computational and Theoretical Chemistry, 2012, 992, 164-167.	2.5	73
33	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.	3.6	73
34	The effect of surface curvature of aluminum nitride nanotubes on the adsorption of NH3. Structural Chemistry, 2011, 22, 1261-1265.	2.0	72
35	Hydrogen dissociation on diene-functionalized carbon nanotubes. Journal of Molecular Modeling, 2013, 19, 255-261.	1.8	72
36	Nitrate adsorption by carbon nanotubes in the vacuum and aqueous phase. Monatshefte FÃ¼r Chemie, 2012, 143, 1623-1626.	1.8	68

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37	Sensing behavior of Al-rich AlN nanotube toward hydrogen cyanide. Journal of Molecular Modeling, 2013, 19, 2197-2203.	1.8	63
38	Carbon nanotube functionalization with carboxylic derivatives: a DFT study. Journal of Molecular Modeling, 2013, 19, 391-396.	1.8	63
39	Theoretical prediction of silicene as a new candidate for the anode of lithium-ion batteries. Physical Chemistry Chemical Physics, 2015, 17, 29689-29696.	2.8	63
40	Functionalization of [60] fullerene with butadienes: A DFT study. Applied Surface Science, 2012, 258, 8980-8984.	6.1	59
41	Boron Nitride Monolayer: A Strain-Tunable Nanosensor. Journal of Physical Chemistry C, 2013, 117, 13261-13267.	3.1	45
42	Hydrogen storage by BeO nano-cage: A DFT study. Applied Surface Science, 2016, 368, 76-81.	6.1	44
43	Induced polarization and electronic properties of carbon-doped boron nitride nanoribbons. Physical Review B, 2012, 86, .	3.2	43
44	Computational study on the characteristics of the interaction in linear urea clusters. International Journal of Quantum Chemistry, 2011, 111, 3184-3195.	2.0	39
45	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.	2.7	37
46	Formaldehyde adsorption on the interior and exterior surfaces of CN nanotubes. Structural Chemistry, 2013, 24, 1331-1337.	2.0	36
47	Nitrous oxide adsorption on pristine and Si-doped AlN nanotubes. Journal of Molecular Modeling, 2013, 19, 943-949.	1.8	36
48	Natural pigments in dye-sensitized solar cell (DSSC): a DFT-TDDFT study. Journal of the Iranian Chemical Society, 2019, 16, 795-805.	2.2	36
49	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	35
50	A computational study of water adsorption on boron nitride nanotube. Structural Chemistry, 2010, 21, 903-908.	2.0	33
51	Exohedral and endohedral adsorption of alkaline earth cations in BN nanocluster. Journal of Molecular Modeling, 2013, 19, 1445-1450.	1.8	33
52	Theoretical 14N nuclear quadrupole resonance parameters for sulfa drugs: Sulfamerazine and sulfathiazole. Journal of Molecular Graphics and Modelling, 2008, 27, 326-331.	2.4	31
53	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
54	Phase transition and mechanical properties of cesium bismuth silver halide double perovskites (Cs₂AgBiX₆, X = Cl, Br, I): a DFT approach. Physical Chemistry Chemical Physics, 2020, 22, 5959-5968.	2.8	30

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55	Reversible structural transition in nanoconfined ice. Physical Review B, 2017, 95, .	3.2	28
56	Preparation of uniform 2D ZnO nanostructures by the ionic liquid-assisted sonochemical method and their optical properties. Ceramics International, 2014, 40, 7769-7774.	4.8	26
57	Electrochemical and DFT study of an anticancer and active anthelmintic drug at carbon nanostructured modified electrode. Materials Science and Engineering C, 2016, 69, 1345-1353.	7.3	26
58	Preparation of Cu2O nanostructures by changing reducing agent and their optical properties. Materials Letters, 2015, 153, 1-4.	2.6	24
59	Effects of functionalization and side defects on single-photon emission in boron nitride quantum dots. Physical Review B, 2017, 96, .	3.2	23
60	First-Principles Study of Water Nanotubes Captured Inside Carbon/Boron Nitride Nanotubes. Langmuir, 2018, 34, 11176-11187.	3.5	23
61	Graphene-silicene bilayer: A nanocapacitor with permanent dipole and piezoelectricity effect. Physical Review B, 2015, 92, .	3.2	20
62	Ultrasonic route synthesis, characterization and electrochemical study of graphene oxide and reduced graphene oxide. Research on Chemical Intermediates, 2019, 45, 487-505.	2.7	20
63	Co-adsorption of CO molecules at the open ends of MgO nanotubes. Structural Chemistry, 2012, 23, 1981-1986.	2.0	19
64	Electro-Optical Properties of Monolayer and Bilayer Pentagonal BN: First Principles Study. Nanomaterials, 2020, 10, 440.	4.1	19
65	Doping effect on the adsorption of NH3 molecule onto graphene quantum dot: From the physisorption to the chemisorption. Journal of Applied Physics, 2013, 114, .	2.5	18
66	Spiral graphone and one-sided fluorographene nanoribbons. Physical Review B, 2013, 87, .	3.2	17
67	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, 7293-7299.	2.8	16
68	Experimental and theoretical study of CO adsorption on the surface of single phase hexagonally plate ZnO. Applied Surface Science, 2014, 315, 8-15.	6.1	14
69	The Alkali Metal Interactions with MgO Nanotubes. Bulletin of the Korean Chemical Society, 2012, 33, 1925-1928.	1.9	14
70	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.	3.0	12
71	Computational study of ammonia adsorption on the perfect and rippled graphene sheet. Physica B: Condensed Matter, 2013, 429, 52-56.	2.7	12
72	Hydrogenated î·-graphene as an ultraviolet optomechanical sensor. RSC Advances, 2020, 10, 26197-26211.	3.6	12

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73	Adsorption of Na, Mg, and Al atoms on BN nanotubes. Thin Solid Films, 2012, 526, 139-142.	1.8	11
74	Effect of nitrogen doping on electronic and optical properties of ZnO sheet: DFT+U study. Computational Condensed Matter, 2018, 15, 1-6.	2.1	11
75	Theoretical study on the functionalization of BC2N nanotube with amino groups. Journal of Molecular Modeling, 2013, 19, 2211-2216.	1.8	10
76	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
77	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.	2.2	9
78	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
79	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.	4.0	9
80	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.	3.7	8
81	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.	2.2	8
82	Toxic CO detection by Li-encapsulated fullerene-like BeO. Structural Chemistry, 2018, 29, 231-241.	2.0	8
83	A density functional study of 15N chemical shielding tensors in quinolines. Chemical Physics Letters, 2009, 476, 196-200.	2.6	7
84	Electronic, magnetic and optical properties of Fe-doped nano-BN sheet: DFT study. Indian Journal of Physics, 2021, 95, 823-831.	1.8	7
85	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.	1.8	6
86	Fundamental mechanisms of hexagonal boron nitride sensing of dopamine, tryptophan, ascorbic acid, and uric acid by first-principles study. Journal of Molecular Modeling, 2022, 28, .	1.8	6
87	The electronic and optical properties of 3d transition metals doped silicene sheet: A DFT study. Materials Research Express, 2019, 6, 126326.	1.6	5
88	Nanoscale investigation of the influence of water on the elastic properties of Câ€“Sâ€“H gel by molecular simulation. Proceedings of the Institution of Mechanical Engineers, Part L: Journal of Materials: Design and Applications, 2019, 233, 1295-1306.	1.1	5
89	A computational study on the BN and AlN nanocones as anode materials for K-ion batteries. Applied Surface Science, 2021, 544, 148793.	6.1	5
90	Electrodeposition of CoxNiVyOz Ternary Nanopetals on Bare and rGO-Coated Nickel Foam for High-Performance Supercapacitor Application. Nanomaterials, 2022, 12, 1894.	4.1	5

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91	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.	3.1	4
92	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	3
93	Synthesis, identification, crystal structure and theoretical study of a Ce(IV) complex. Journal of the Iranian Chemical Society, 2014, 11, 1353-1361.	2.2	3
94	Boron nitride nanochannels encapsulating a water/heavy water layer for energy applications. RSC Advances, 2019, 9, 5901-5907.	3.6	3
95	Theoretical investigation of azo dyes adsorbed on cellulose fibers: 1. Electronic and bonding structures. Journal of the Iranian Chemical Society, 2013, 10, 985-999.	2.2	2
96	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.	2.2	2
97	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.	2.2	2
98	Theoretical investigation of azo dyes adsorbed on cellulose fibers: 2. Spectroscopic study. Journal of the Iranian Chemical Society, 2014, 11, 111-121.	2.2	1
99	Experimental and Theoretical Study of Porous Al2O3. Transactions of the Indian Institute of Metals, 2021, 74, 381-386.	1.5	1
100	Investigation of Interaction Between Graphene and Its Compounds as Carriers on Anti-Cancer Drug of 5-Fluorouracil. Eurasian Journal of Analytical Chemistry, 2018, 13, .	0.4	1
101	Effect of vacancy modification on the quantum capacitance of silicene- based electrode in efficient supercapacitors. Thin Solid Films, 2022, 756, 139378.	1.8	1
102	A Theoretical Model Based on Modified Fullerenes for Photodynamic Therapy of Cancer. Journal of Computational and Theoretical Nanoscience, 2018, 15, 147-152.	0.4	0