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	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
2	Electrodeposition of CoxNiVyOz Ternary Nanopetals on Bare and rGO-Coated Nickel Foam for High-Performance Supercapacitor Application. Nanomaterials, 2022, 12, 1894.	4.1	5
3	Effect of vacancy modification on the quantum capacitance of silicene- based electrode in efficient supercapacitors. Thin Solid Films, 2022, 756, 139378.	1.8	1
4	Electronic, magnetic and optical properties of Fe-doped nano-BN sheet: DFT study. Indian Journal of Physics, 2021, 95, 823-831.	1.8	7
5	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
6	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
7	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
8	Experimental and Theoretical Study of Porous Al2O3. Transactions of the Indian Institute of Metals, 2021, 74, 381-386.	1.5	1
9	Hydrogenated Î¨-graphene as an ultraviolet optomechanical sensor. RSC Advances, 2020, 10, 26197-26211.	3.6	12
10	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
11	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
12	Electro-Optical Properties of Monolayer and Bilayer Pentagonal BN: First Principles Study. Nanomaterials, 2020, 10, 440.	4.1	19
13	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
14	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
15	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
16	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
17	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
18	Boron nitride nanochannels encapsulating a water/heavy water layer for energy applications. RSC Advances, 2019, 9, 5901-5907.	3.6	3

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19	The electronic and optical properties of 3d transition metals doped silicene sheet: A DFT study. Materials Research Express, 2019, 6, 126326.	1.6	5
20	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
21	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
22	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
23	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
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	Toxic CO detection by Li-encapsulated fullerene-like BeO. Structural Chemistry, 2018, 29, 231-241.	2.0	8
26	First-Principles Study of Water Nanotubes Captured Inside Carbon/Boron Nitride Nanotubes. Langmuir, 2018, 34, 11176-11187.	3.5	23
27	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
28	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
29	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
30	Reversible structural transition in nanoconfined ice. Physical Review B, 2017, 95, .	3.2	28
31	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
32	Effects of functionalization and side defects on single-photon emission in boron nitride quantum dots. Physical Review B, 2017, 96, .	3.2	23
33	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
34	Van der Waals pressure and its effect on trapped interlayer molecules. Nature Communications, 2016, 7, 12168.	12.8	137
35	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
36	Hydrogen storage by BeO nano-cage: A DFT study. Applied Surface Science, 2016, 368, 76-81.	6.1	44

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37	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
38	Microporous titaniaâ€“silica nanocomposite catalyst-adsorbent for ultra-deep oxidative desulfurization. Applied Catalysis B: Environmental, 2016, 180, 65-77.	20.2	153
39	Graphene-silicene bilayer: A nanocapacitor with permanent dipole and piezoelectricity effect. Physical Review B, 2015, 92, .	3.2	20
40	Preparation of Cu2O nanostructures by changing reducing agent and their optical properties. Materials Letters, 2015, 153, 1-4.	2.6	24
41	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
42	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
43	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
44	Density-functional calculations of HCN adsorption on the pristine and Si-doped graphynes. Structural Chemistry, 2014, 25, 1-7.	2.0	79
45	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
46	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
47	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
48	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
49	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
50	Formaldehyde adsorption on the interior and exterior surfaces of CN nanotubes. Structural Chemistry, 2013, 24, 1331-1337.	2.0	36
51	Ab initio study of NH3 and H2O adsorption on pristine and Na-doped MgO nanotubes. Structural Chemistry, 2013, 24, 165-170.	2.0	80
52	Sensing behavior of Al-rich AlN nanotube toward hydrogen cyanide. Journal of Molecular Modeling, 2013, 19, 2197-2203.	1.8	63
53	Computational study of ammonia adsorption on the perfect and rippled graphene sheet. Physica B: Condensed Matter, 2013, 429, 52-56.	2.7	12
54	DFT study on the functionalization of a BN nanotube with sulfamide. Applied Surface Science, 2013, 266, 182-187.	6.1	87

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55	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
56	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
57	Hydrogen dissociation on diene-functionalized carbon nanotubes. Journal of Molecular Modeling, 2013, 19, 255-261.	1.8	72
58	Carbon nanotube functionalization with carboxylic derivatives: a DFT study. Journal of Molecular Modeling, 2013, 19, 391-396.	1.8	63
59	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
60	Nitrous oxide adsorption on pristine and Si-doped AlN nanotubes. Journal of Molecular Modeling, 2013, 19, 943-949.	1.8	36
61	Sensing behavior of Al and Si doped BC3 graphenes to formaldehyde. Sensors and Actuators B: Chemical, 2013, 181, 829-834.	7.8	188
62	Spiral graphone and one-sided fluorographene nanoribbons. Physical Review B, 2013, 87, .	3.2	17
63	Ammonia monitoring by carbon nitride nanotubes: A density functional study. Thin Solid Films, 2013, 534, 650-654.	1.8	75
64	Exohedral and endohedral adsorption of alkaline earth cations in BN nanocluster. Journal of Molecular Modeling, 2013, 19, 1445-1450.	1.8	33
65	Theoretical study on the functionalization of BC2N nanotube with amino groups. Journal of Molecular Modeling, 2013, 19, 2211-2216.	1.8	10
66	Boron Nitride Monolayer: A Strain-Tunable Nanosensor. Journal of Physical Chemistry C, 2013, 117, 13261-13267.	3.1	45
67	Carbon nitride nanotube as a sensor for alkali and alkaline earth cations. Applied Surface Science, 2013, 264, 699-706.	6.1	82
68	B12N12 Nano-cage as Potential Sensor for NO2 Detection. Chinese Journal of Chemical Physics, 2012, 25, 60-64.	1.3	126
69	Nitrate adsorption by carbon nanotubes in the vacuum and aqueous phase. Monatshefte FÃ¼r Chemie, 2012, 143, 1623-1626.	1.8	68
70	Electronic sensor for sulfide dioxide based on AlN nanotubes: a computational study. Journal of Molecular Modeling, 2012, 18, 4745-4750.	1.8	80
71	Induced polarization and electronic properties of carbon-doped boron nitride nanoribbons. Physical Review B, 2012, 86, .	3.2	43
72	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

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73	Theoretical study of CO adsorption on the surface of BN, AlN, BP and AlP nanotubes. Surface Science, 2012, 606, 981-985.	1.9	152
74	Adsorption and dissociation of Cl2 molecule on ZnO nanocluster. Applied Surface Science, 2012, 258, 8171-8176.	6.1	117
75	Functionalization of [60] fullerene with butadienes: A DFT study. Applied Surface Science, 2012, 258, 8980-8984.	6.1	59
76	Quantum chemical study of fluorinated AlN nano-cage. Applied Surface Science, 2012, 259, 631-636.	6.1	97
77	Selective function of Al12N12 nano-cage towards NO and CO molecules. Computational Materials Science, 2012, 62, 71-74.	3.0	136
78	Theoretical investigation of C60 fullerene functionalization with tetrazine. Computational and Theoretical Chemistry, 2012, 992, 164-167.	2.5	73
79	Theoretical study of hydrogen adsorption on the B12P12 fullerene-like nanocluster. Computational Materials Science, 2012, 54, 115-118.	3.0	95
80	Adsorption of Na, Mg, and Al atoms on BN nanotubes. Thin Solid Films, 2012, 526, 139-142.	1.8	11
81	Detection of phosgene by Sc-doped BN nanotubes: A DFT study. Sensors and Actuators B: Chemical, 2012, 171-172, 846-852.	7.8	292
82	Interaction of small molecules (NO, H2, N2, and CH4) with BN nanocluster surface. Structural Chemistry, 2012, 23, 1567-1572.	2.0	103
83	Co-adsorption of CO molecules at the open ends of MgO nanotubes. Structural Chemistry, 2012, 23, 1981-1986.	2.0	19
84	A theoretical study of CO adsorption on aluminum nitride nanotubes. Structural Chemistry, 2012, 23, 653-657.	2.0	77
85	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
86	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
87	A comparative study on the B12N12, Al12N12, B12P12 and Al12P12 fullerene-like cages. Journal of Molecular Modeling, 2012, 18, 2653-2658.	1.8	160
88	AlN nanotube as a potential electronic sensor for nitrogen dioxide. Microelectronics Journal, 2012, 43, 452-455.	2.0	96
89	The Alkali Metal Interactions with MgO Nanotubes. Bulletin of the Korean Chemical Society, 2012, 33, 1925-1928.	1.9	14
90	Toxic CO detection by B12N12 nanocluster. Microelectronics Journal, 2011, 42, 1400-1403.	2.0	124

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91	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
92	Chemisorption of NH3 at the open ends of boron nitride nanotubes: a DFT study. Structural Chemistry, 2011, 22, 183-188.	2.0	88
93	The effect of surface curvature of aluminum nitride nanotubes on the adsorption of NH3. Structural Chemistry, 2011, 22, 1261-1265.	2.0	72
94	Computational study on the characteristics of the interaction in linear urea clusters. International Journal of Quantum Chemistry, 2011, 111, 3184-3195.	2.0	39
95	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
96	Interaction of NH3 with aluminum nitride nanotube: Electrostatic vs. covalent. Physica E: Low-Dimensional Systems and Nanostructures, 2011, 43, 1717-1719.	2.7	84
97	A computational study of water adsorption on boron nitride nanotube. Structural Chemistry, 2010, 21, 903-908.	2.0	33
98	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
99	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
100	A density functional study of 15N chemical shielding tensors in quinolines. Chemical Physics Letters, 2009, 476, 196-200.	2.6	7
101	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
102	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