Maziar Noei

List of Publications by Year
in descending order

51 papers	1,197 citations	394421 19 h-index	377865 34 g-index
51 all docs	51 docs citations	51 times ranked	724 citing authors

#	Article	IF	Citations
1	Al-doped graphene-like BN nanosheet as a sensor for para-nitrophenol: DFT study. Superlattices and Microstructures, 2013, 59, 115-122.	3.1	185
2	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
3	The alkali and alkaline earth metal doped ZnO nanotubes: DFT studies. Physica B: Condensed Matter, 2014, 432, 105-110.	2.7	81
4	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
5	Ammonia monitoring by carbon nitride nanotubes: A density functional study. Thin Solid Films, 2013, 534, 650-654.	1.8	75
6	A DFT study on the sensing behavior of a BC2N nanotube toward formaldehyde. Journal of Molecular Modeling, 2013, 19, 3843-3850.	1.8	63
7	DFT study of the dissociative adsorption of HF on an AlN nanotube. Comptes Rendus Chimie, 2013, 16, 985-989.	0.5	58
8	Aluminum nitride nanotubes. Chemical Papers, 2017, 71, 881-893.	2.2	51
9	DFT study on the sensitivity of open edge graphene toward CO2 gas. Vacuum, 2016, 131, 194-200.	3.5	49
10	Adsorption of Formic Acid and Formate Anion on ZnO Nanocage: A DFT Study. Journal of Cluster Science, 2015, 26, 609-621.	3.3	43
11	Removal of ethyl acetylene toxic gas from environmental systems using AlN nanotube. Journal of Nanostructure in Chemistry, 2015, 5, 213-217.	9.1	41
12	Different electronic sensitivity of BN and AlN nanoclusters to SO2 gas: DFT studies. Vacuum, 2017, 135, 44-49.	3.5	38
13	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
14	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
15	Hydrogen fluoride on the pristine, Al and Si doped BC2N nanotubes: A computational study. Computational Materials Science, 2014, 82, 197-201.	3.0	27
16	Functionalization of the pristine and stone-wales defected BC3 graphenes with pyrene. Journal of Molecular Modeling, 2014, 20, 2539.	1.8	25
17	Working Mechanism of a BC ₃ Nanotube Carbon Monoxide Gas Sensor. Communications in Theoretical Physics, 2013, 60, 113-118.	2.5	24
18	Fluorination of BC3 nanotubes: DFT studies. Journal of Molecular Modeling, 2013, 19, 3941-3946.	1.8	23

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19	Ethyl benzene detection by BN nanotube: DFT studies. Journal of Saudi Chemical Society, 2017, 21, S12-S16.	5.2	23
20	Tunable Bandgap in Bilayer Armchair Graphene Nanoribbons: Concurrent Influence of Electric Field and Uniaxial Strain. IEEE Transactions on Electron Devices, 2013, 60, 2464-2470.	3.0	19
21	Probing the electronic sensitivity of BN and carbon nanotubes to carbonyl sulfide: A theoretical study. Journal of Molecular Liquids, 2016, 224, 757-762.	4.9	17
22	Facile synthesis of N-(arylsulfonyl)-4-ethoxy-5-oxo-2,5-dihydro-1H-pyrolle-2,3-dicarboxylates by one-pot three-component reaction. Chinese Chemical Letters, 2012, 23, 45-48.	9.0	16
23	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
24	The effect of electric field on the cell voltage of inorganic AlN nanosheet based Naâ€“ion batteries. Inorganic Chemistry Communication, 2018, 91, 29-34.	3.9	11
25	Adsorption properties of CH3COOH on (6,0), (7,0), and (8,0) zigzag, and (4,4), and (5,5) armchair single-walled carbon nanotubes: A density functional study. Arabian Journal of Chemistry, 2017, 10, S3001-S3006.	4.9	9
26	DFT study on [4+2] and [2+2] cycloadditions to [60] fullerene. Chemical Papers, 2014, 68, .	2.2	8
27	Organometallic compound as an efficient catalyst toward oxygen reduction reaction. Inorganic Chemistry Communication, 2019, 108, 107520.	3.9	8
28	Evaluating Minnesota 2006 density functionals against some challenging problems in DFT. Journal of Molecular Modeling, 2017, 23, 38.	1.8	7
29	The ab initio study and NBO interpretation of solvent effects on the structural stability and the chemical reactivity of penicillin-V conformations. Arabian Journal of Chemistry, 2017, 10, S2327-S2334.	4.9	7
30	Novel Efficient Three-Component, One-Pot Synthesis of 3-(Î±-amidobenzyl)-4-hydroxycoumarin derivatives. Journal of Chemical Research, 2012, 36, 715-717.	1.3	6
31	Potential application of AlN nanostructures in sodium ion batteries: a DFT study. Molecular Physics, 2019, 117, 359-367.	1.7	6
32	A Facile Synthesis of Polysubstituted Pyrroles by One-Pot Three-Component Reaction. E-Journal of Chemistry, 2012, 9, 2239-2244.	0.5	5
33	Density functional study on the sensing properties of nano-sized BeO tube toward H2S. Journal of the Iranian Chemical Society, 2014, 11, 725-731.	2.2	5
34	TM-CmHm organometallics (TM=Fe, Co, Ni, Cu, Zn and m=4, 5, 6) for highly efficient Pt-free catalytic activation of O2 molecule. Journal of Molecular Structure, 2020, 1200, 127008.	3.6	5
35	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
36	Pyrrole adsorption on aluminum nitride nanotubes on DFT data. Russian Journal of Physical Chemistry A, 2016, 90, 2221-2229.	0.6	4

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37	A computational study on the BN-yne sheet application in the Na-ion batteries. Journal of Molecular Graphics and Modelling, 2020, 97, 107567.	2.4	4
38	Selective Sensing Characteristics of Ca Doped BeO Nanoâ€sized Tube toward H2O and NH3. Chinese Journal of Chemical Physics, 2013, 26, 612-616.	1.3	3
39	A theoretical study on monoatomic BN nanochains and nanorings. Journal of Molecular Modeling, 2016, 22, 205.	1.8	3
40	Design of methyldopa structure and calculation of its properties by quantum mechanics. Arabian Journal of Chemistry, 2017, 10, S1923-S1937.	4.9	3
41	Theoretical study of the catalytic effect of TM-C4H4 and TM-C5H5 (TMÂ=ÂCr, Ti, V, Sc) on the activation of O2 at the cathode and CH3OH at the anode in â€œCH3OH-O2â€³ fuel cell via DFT computational method. Arabian Journal of Chemistry, 2021, 14, 103062.	4.9	3
42	Enhanced gas permeation performance of mixed matrix membranes containing polysulfone and modified mesoporous MCM-41. Journal of the Serbian Chemical Society, 2021, 86, 871-887.	0.8	2
43	Density functional theory study on the [5,6]-diaryl-methano fulleroids of C 70 with different functional groups. Vacuum, 2016, 134, 48-53.	3.5	1
44	Theoretical study of activation of O 2 at cathode and CH 3 OH at anode of â€œ CH 3 OH â€•O 2 â€•fuel cell using ZnC 4 H 4 and. Journal of the Chinese Chemical Society, 2021, 68, 793-798.	1.4	1
45	CHARACTERIZATION OF ELECTRONIC STRUCTURES ON THE ADSORPTION BEHAVIORS OF MERCAPTOPURINE ANTICANCER DRUG FROM SURFACE MACROMOLECULE CALIX[4]AREN AS ADSORBENT BY SPECTRAL STUDIES AND DFT CALCULATIONS. Surface Review and Letters, 2022, 29, .	1.1	1
46	Alkali metal ions on a nanosized tube of BC2N: Computational study. Physica E: Low-Dimensional Systems and Nanostructures, 2014, 56, 90-95.	2.7	0
47	The Catalytic Effect of Organometallic Compounds on Oxygen-Hydrazine Fuel Cell: A DFT Study. Russian Journal of Physical Chemistry A, 2021, 95, 1581-1584.	0.6	0
48	Theoretical study of the catalytic effect of TM-CmHm (TMâ€‰=â€‰Cr, Mn, Sc, Ti, V, and mâ€‰=â€‰4, 5) on the activation of oxygen at the cathode and methane at the anode in the fuel cell reaction â€œCH4â€“O2â€• a DFT study. Structural Chemistry, 0, , 1.	2.0	0
49	New structure-based models for the prediction of normal boiling point temperature of ternary azeotropes. Journal of the Serbian Chemical Society, 2021, 86, 685-698.	0.8	0
50	Experimental evaluation of free chlorine adsorption from circulating water in cooling towers by activated carbon in a fixed bed column. Revue Roumaine De Chimie, 2021, 65, 1067-1077.	0.2	0
51	The Effect of Organometallic Compounds and â€œOxygenâ€“Methaneâ€•Fuel Cell: A DFT Study. Russian Journal of Physical Chemistry A, 2021, 95, 2229-2233.	0.6	0