Zabiollah Mahdavifar

List of Publications by Citations

44 papers	526 citations	15 h-index	20 g-index
44 ext. papers	586 ext. citations	4.2 avg, IF	4.53 L-index

#	Paper	IF	Citations
44	Theoretical study of the inclusion complexes of α- and β-cyclodextrins with decyltrimethylammonium bromide (DTAB) and tetradecyltrimethylammonium bromide (TTAB). *Journal of Molecular Liquids*, **2007**, 135, 153-157	6	39
43	Theoretical prediction of ozone sensing using pristine and endohedral metalloboron B80 fullerenes. *Sensors and Actuators B: Chemical*, **2014**, 205, 26-38	8.5	33
42	A comparative theoretical study of CO2 sensing using inorganic AlN, BN and SiC single walled nanotubes. *Sensors and Actuators B: Chemical*, **2013**, 185, 512-522	8.5	32
41	Four-coordinate and pseudo five-coordinate Hg(II) complexes of a new bidentate phosphorus ylide: X-ray crystal structure and spectral characterization. *Journal of Organometallic Chemistry*, **2010**, 695, 1441-1450	2.3	26
40	Electronic Properties of Adsorption Nitrogen Monoxide on Inside and Outside of the Armchair Single Wall Carbon Nanotubes: A Density Functional Theory Calculations. *Journal of Physical Chemistry C*, **2008**, 112, 3597-3604	3.8	25
39	Theoretical investigation of pristine and functionalized AlN and SiC single walled nanotubes as an adsorption candidate for methane. *Applied Surface Science*, **2012**, 263, 553-562	6.7	24
38	Theoretical approach into potential possibility of efficient NO2 detection via B40 and Li@B40 fullerenes. *Chemical Physics Letters*, **2018**, 691, 360-365	2.5	23
37	Stability prediction of pristine and metal endohedral borofullerenes: Computational approach. *Journal of Molecular Liquids*, **2016**, 219, 1144-1156	6	22
36	Theoretical prediction of encapsulation and adsorption of platinum-anticancer drugs into single walled boron nitride and carbon nanotubes. *Journal of Inclusion Phenomena and Macrocyclic Chemistry*, **2014**, 79, 443-457	1.7	22
35	Canonical Monte Carlo simulation of adsorption of O2 and N2 mixture on single walled carbon nanotube at different temperatures and pressures. *Journal of Computational Chemistry*, **2010**, 31, 1443-9	3.5	22
34	Synthesis, characterization, and structural studies of mercury(II) complexes of new bidentate phosphorus ylide. *Inorganica Chimica Acta*, **2010**, 363, 1254-1261	2.7	22
33	Preference prediction for the stable inclusion complex formation between cucurbit [n = 5–7]urils with anticancer drugs based on platinum (II): Computational study. *Journal of Molecular Liquids*, **2012**, 166, 53-61	6	21
32	The influence of Cu-doping on aluminum nitride, silicon carbide and boron nitride nanotubes' ability to detect carbon dioxide; DFT study. *Physica E: Low-Dimensional Systems and Nanostructures*, **2014**, 56, 268-276	3	19
31	Effect of the adsorption of oxygen on electronic structures and geometrical parameters of armchair single-wall carbon nanotubes: a density functional study. *Journal of Colloid and Interface Science*, **2009**, 336, 1-12	9.3	17
30	New mononuclear mercury(II) complexes of a bifunctionalized ylide containing five-membered chelate ring: Spectral and structural characterization. *Inorganica Chimica Acta*, **2010**, 363, 3654-3661	2.7	16
29	Synthesis of new phosphorus ylides: Spectroscopic and X-ray structural studies. *Heteroatom Chemistry*, **2010**, 21, 475-485	1.2	15
28	Theoretical prediction of maximum capacity of C- and Si-fullerenes for noble gas storage. *Journal of Molecular Graphics and Modelling*, **2014**, 54, 32-45	2.8	13

27	Predicting helium and neon adsorption and separation on carbon nanotubes by Monte Carlo simulation. *Journal of Molecular Modeling*, **2011**, 17, 785-94	2	13
26	Evolutionary search for (M B) (M = Sc-Ni; Q = 0/-1) clusters: bowl/boat vs. tubular shape. *Physical Chemistry Chemical Physics*, **2019**, 21, 22618-22628	3.6	13
25	Hetero-fullerenes C59M (M = B, Al, Ga, Ge, N, P, As) for sulfur dioxide gas sensing: Computational approach. *Chemical Physics*, **2020**, 530, 110606	2.3	10
24	Evaluation of photovoltaic properties and effective conjugated length of DTTTD-based polymers as donor in BHJ solar cells; quantum chemical approach. *Polymer*, **2017**, 126, 162-176	3.9	9
23	Thermodynamic studies of inclusion complex formation between alkylpyridinium chlorides and Cyclodextrin using conductometric method. *Journal of Inclusion Phenomena and Macrocyclic Chemistry*, **2010**, 67, 247-252		8
22	Can Fluorine form Halogen Bond? Investigation of Halogen Bonds through Steric Charge. *ChemistrySelect*, **2017**, 2, 2713-2717	1.8	7
21	Theoretical investigation of inclusion complex formation of Gold (III) Dimethyldithiocarbamate anticancer agents with cucurbit[n=5,6]urils. *Arabian Journal of Chemistry*, **2014**, 7, 425-435	5.9	7
20	CdInGaS4: An unexplored two- dimensional materials with desirable band gap for optoelectronic devices. *Journal of Alloys and Compounds*, **2021**, 854, 157220	5.7	7
19	Copper halide diselenium: predicted two-dimensional materials with ultrahigh anisotropic carrier mobilities.. *RSC Advances*, **2020**, 10, 8016-8026	3.7	5
18	Electro-Optical Properties and Structural Stability Perspectives of M3N and M2C2 (M = Sc, La) Clusters Encapsulated in B80 Fullerene: A Density Functional Theory Study. *Journal of Electronic Materials*, **2018**, 47, 550-565	1.9	5
17	Tuning of Elastic Properties of Nanotubes by Imposing a Transverse Electric Field: Computational Approach. *Journal of Physical Chemistry C*, **2016**, 120, 17801-17809	3.8	5
16	Modifying the electronic and geometrical properties of mono/bi-layer graphite-like BC2N via alkali metal (Li, Na) adsorption and intercalation: computational approach. *New Journal of Chemistry*, **2019**, 43, 13122-13133	3.6	5
15	Theoretical investigation of ethane and ethene monitoring using pristine and decorated aluminum nitride and silicon carbide nanotubes. *Sensors and Actuators B: Chemical*, **2014**, 196, 555-566	8.5	5
14	Theoretical studies of n-membered ring chelate complexes of Ni(II), Pd(II) and Pt(II) derived from bidentate phosphorus ylides. *Polyhedron*, **2014**, 72, 72-82	2.7	5
13	Electronic and stability characters of endohedral Zn@Sin and exohedral SinHn (n = 20, 30, 40, 50, 60) fullerenes: A DFT approach. *Journal of Molecular Liquids*, **2016**, 219, 561-572	6	5
12	Exploring the electro-optical properties of conjugated polymers based on oligo-selenophene and oligo(3,4-ethylenedioxyselenophene). *Applied Organometallic Chemistry*, **2019**, 33, e4962	3.1	4
11	Carbon monoxide monitoring using pristine and Cu-functionalized aluminum nitride and silicon carbide nanotubes; DFT study. *Journal of Molecular Liquids*, **2015**, 204, 147-155	6	4
10	Systematic investigation of structure and optoelectronic properties of Ge (n B20), MGe9 (M Ga, Si, Sn, As) and GaxGe(10) (x 1 10) Clusters: Computational approach. *Polyhedron*, **2021**, 193, 114874	2.7	4

9	Umbrella-shaped vs planar; evolutionary search for BnQ, Be BnQ (n = 6 12, Q = 0, 1) clusters. *Journal of Molecular Liquids*, **2021**, 328, 115389	6	3
8	Prediction of unexpected BnPn structures: promising materials for non-linear optical devices and photocatalytic activities. *Nanoscale Advances*, **2021**, 3, 2846-2861	5.1	3
7	A quantum chemical study of the factors influencing performance of DTTTD: Fullerene hetrojunction photovoltaic models. *Journal of Photochemistry and Photobiology A: Chemistry*, **2015**, 310, 9-25	4.7	2
6	Exploring the optical and nonlinear optical features of heteroleptic complexes with BODIPY and amido-BODIPY substitutions; A comparative theoretical study. *Inorganic Chemistry Communication*, **2020**, 121, 108234	3.1	2
5	Prediction of beryllium clusters (Be; = 3-25) from first principles. *Physical Chemistry Chemical Physics* , **2021**, 23, 19716-19728	3.6	2
4	Different coordination modes of bifunctionalized ylides in complexation with group 12 metals via computational approach. *Journal of Molecular Liquids*, **2016**, 219, 579-591	6	1
3	Length dependence of conductance in benzothiadiazole molecular wires between graphene nanoribbon electrodes: Effect of conformational changes. *Journal of Molecular Liquids*, **2018**, 269, 639-649	6	1
2	Response surface methodology optimizing the adsorptive removal of azithromycin using mesoporous silica SBA-15: Mechanism, thermodynamic, equilibrium, and kinetics modeling studies. *Journal of Environmental Science and Health - Part A Toxic/Hazardous Substances and Environmental Engineering*, **2021**, 56, 1145-1164	2.3	0
1	Achieved negative differential resistance behavior of Si/B-substituted into a C chain sandwiched between capped carbon nanotube junctions.. *RSC Advances*, **2022**, 12, 1758-1768	3.7	