Ehsan Shakerzadeh

List of Publications by Year
in descending order

61 papers	1,384 citations	361413 20 h-index	377865 34 g-index
61 all docs	61 docs citations	61 times ranked	937 citing authors

#	Article	IF	Citations
1	A comparative DFT study on prospective application of C24, Si12C12, B12N12, B12P12, Al12N12, and Al12P12 nanoclusters as suitable anode materials for magnesium-ion batteries (MIBs). Physica E: Low-Dimensional Systems and Nanostructures, 2022, 140, 115161.	2.7	16
2	Acetylsalicylic acid interaction with Boron nitride nanostructures â€“ A density functional analysis. Journal of Molecular Liquids, 2022, 355, 118980.	4.9	21
3	Pristine and alkali and alkaline earth metals encapsulated B₃₆N₃₆ nanoclusters as prospective delivery agents and detectors for 5â€fluorouracil anticancer drug. Applied Organometallic Chemistry, 2022, 36, .	3.5	22
4	Magnesiation of bare and halides encapsulated B40 fullerenes for their potential application as promising anode materials for Mg-ion batteries. Applied Surface Science, 2021, 538, 148060.	6.1	27
5	Can C24N24 cavernous nitride fullerene be a potential anode material for Li-, Na-, K-, Mg-, Ca-ion batteries?. Chemical Physics Letters, 2021, 764, 138241.	2.6	22
6	Synthesis, structural characterization, and density functional theory calculations of the two new Zn (II) complexes as antibacterial and anticancer agents with a neutral flexible tetradentate pyrazoleâ€based ligand. Applied Organometallic Chemistry, 2021, 35, e6173.	3.5	18
7	Efficient carriers for anticancer 5-fluorouracil drug based on the bare and Mâ^'encapsulated (Mâ€¯=â€¯Na) Tj ETQq1 1 0.784314 rgBT	4.9	24
8	Li@B40 and Na@B40 fullerenes serving as efficient carriers for anticancer nedaplatin drug: A quantum chemical study. Computational and Theoretical Chemistry, 2021, 1202, 113339.	2.5	17
9	Ngn (Ng= Ne, Ar, Kr, Xe, and Rn; n=1, 2) encapsulated porphyrin-like porous C24N24 fullerene: A quantum chemical study. Journal of Molecular Graphics and Modelling, 2021, 108, 107986.	2.4	30
10	Hetero-fullerenes C59M (Mâ€¯=â€¯B, Al, Ga, Ge, N, P, As) for sulfur dioxide gas sensing: Computational approach. Chemical Physics, 2020, 530, 110606.	1.9	11
11	Electronic and nonlinear optical features of first row transition metals-decorated all-boron B40 fullerene: A promising route to remarkable electro-optical response. Inorganic Chemistry Communication, 2020, 112, 107692.	3.9	15
12	Enhanced electronic and nonlinear optical responses of C₂₄N₂₄ cavernous nitride fullerene by decoration with first row transition metals; A computational investigation. Applied Organometallic Chemistry, 2020, 34, e5694.	3.5	23
13	The teetotum cluster Li₂FeB₁₄and its possible use for constructing boron nanowires. Physical Chemistry Chemical Physics, 2020, 22, 15013-15021.	2.8	3
14	Fe-decorated all-boron B40 fullerene serving as a potential promising active catalyst for CO oxidation: A DFT mechanistic approach. Polyhedron, 2020, 188, 114699.	2.2	16
15	Exploring enthalpies of formation of imidazolium-, pyridinium-, and pyrrolidinium-based ionic liquids with dicyanamide anion using quantum chemical methods. Journal of Molecular Liquids, 2020, 308, 113137.	4.9	6
16	The Al, Ga and Sc dopants effect on the adsorption performance of B12N12 nanocluster toward pnictogen hydrides. Chemical Physics, 2019, 526, 110424.	1.9	37
17	Functionalized olympicene (C19H12) as anode material for Li-ion batteries: a DFT approach. Monatshefte FÃ¼r Chemie, 2019, 150, 1745-1751.	1.8	6
18	Electro-optical properties of bowl-like B36 cluster doped with the first row transition metals: A DFT insight. Physica E: Low-Dimensional Systems and Nanostructures, 2019, 114, 113599.	2.7	17

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19	Computational mechanistic insights into CO oxidation reaction over Fe decorated C24N24 fullerene. Inorganic Chemistry Communication, 2019, 106, 190-196.	3.9	26
20	Exploring the electroâ€optical properties of conjugated polymers based on oligoâ€selenophene and oligo(3,4â€ethylenedioxyselenophene). Applied Organometallic Chemistry, 2019, 33, e4962.	3.5	4
21	A DFT study on the potential application of Si@C24N24 porous fullerene as an innovative and highly active catalyst for NO reduction. Chemical Physics Letters, 2019, 724, 80-85.	2.6	19
22	The scandium doped boron cluster B₂₇Sc₂⁺: a fruit can-like structure. Physical Chemistry Chemical Physics, 2019, 21, 8933-8939.	2.8	14
23	Tuning the electronicâ€optical properties of porphyrinâ€like porous C₂₄N₂₄ fullerene with (Li₃O)_{nÂ=Â(1â€“5)} decoration. A computational study. Applied Organometallic Chemistry, 2019, 33, e4654.	3.5	9
24	How Does Lithiation Affect Electro-Optical Features of Corannulene (C20H10) and Quadrannulene (C16H8) Buckybowls?. Journal of Electronic Materials, 2018, 47, 2348-2358.	2.2	22
25	Theoretical approach into potential possibility of efficient NO2 detection via B40 and Li@B40 fullerenes. Chemical Physics Letters, 2018, 691, 360-365.	2.6	27
26	Silicon carbide nanotubes (SiCNTs) serving for catalytic decomposition of toxic diazomethane (DAZM) gas: a DFT study. Molecular Physics, 2018, 116, 414-422.	1.7	3
27	Probing the adsorption behavior of oxazole and isoxazole heterocyclic compounds onto B₁₂N₁₂ nanocluster surface in gas and aqueous mediums through DFT calculations. Applied Organometallic Chemistry, 2018, 32, e4543.	3.5	5
28	Tailoring C24S12 and C16S8 sulflowers with lithium atom for the remarkable first hyperpolarizability. Chemical Physics Letters, 2018, 709, 33-40.	2.6	10
29	Computational evaluation of the remarkable electro-optical responses of the multilithiated pristine and heterosubstituted sumanenes. Chemical Physics Letters, 2017, 678, 51-58.	2.6	8
30	Quantum chemical assessment of the adsorption behavior of fluorouracil as an anticancer drug on the B 36 nanosheet. Journal of Molecular Liquids, 2017, 240, 682-693.	4.9	29
31	In silico investigation of the ozone (O3) binding behavior to the B36 bowl-shaped structure. Adsorption, 2017, 23, 879-886.	3.0	9
32	A computational study on the electro-optical characteristics of C 2n (BN) 12-n (n = 1â€“11) hetero-nanoclusters: Toward the remarkable features by the encapsulation via alkali metals. Journal of Molecular Liquids, 2017, 233, 236-242.	4.9	4
33	Li n @B36 (nÂ=Â1, 2) Nanosheet with Remarkable Electro-Optical Properties: A DFT Study. Journal of Electronic Materials, 2017, 46, 4420-4425.	2.2	14
34	Electronic and nonlinear optical characteristics of the LiB n (n = 4â€“11) nanoclusters: A theoretical study. Microelectronic Engineering, 2017, 183-184, 64-68.	2.4	7
35	Quantum chemical description of formaldehyde (HCHO), acetaldehyde (CH3CHO) and propanal (CH3CH2CHO) pollutants adsorption behaviors onto the bowl-shaped B36 nanosheet. Adsorption, 2017, 23, 1041-1053.	3.0	9
36	Theoretical insight into the impact of sumanene functionalization with BH and NH groups on its ozone addition features. Vacuum, 2017, 136, 82-90.	3.5	11

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37	Synthesis, structural characterization, antibacterial activity, DNA binding and computational studies of bis(2-methyl-1H-imidazole Î²N3)silver(I)dichromate(VI). Journal of Molecular Structure, 2017, 1133, 591-606.	3.6	12
38	Theoretical investigations of interactions between boron nitride nanotubes and drugs. , 2016, , 59-77.		9
39	Selective detection of toxic cyanogen gas in the presence of O 2 , and H 2 O molecules using a AlN nanocluster. Physics Letters, Section A: General, Atomic and Solid State Physics, 2016, 380, 2854-2860.	2.1	12
40	M@B40 (M = Li, Na, K) serving as a potential promising novel NLO nanomaterial. Chemical Physics Letters, 2016, 654, 76-80.	2.6	71
41	Nonlinear Optical (NLO) Response of Pristine and Functionalized Dodecadehydrotribenzo[18]annulene ([18]DBA): A Theoretical Study. Bulletin of the Chemical Society of Japan, 2016, 89, 692-699.	3.2	25
42	A quantum chemical study on the remarkable nonlinear optical and electronic characteristics of boron nitride nanoclusters by complexation via lithium atom. Journal of Molecular Liquids, 2016, 221, 443-451.	4.9	32
43	Sensing of ozone (O3) molecule via pristine singe-walled aluminum nitride nanotube: A DFT study. Superlattices and Microstructures, 2016, 89, 390-397.	3.1	8
44	Theoretical assessment of phosgene adsorption behavior onto pristine, Al- and Ga-doped B12N12 and B16N16 nanoclusters. Computational Materials Science, 2016, 118, 155-171.	3.0	45
45	Theoretical assessment of the electro-optical features of the group III nitrides (B12N12, Al12N12 and) Tj ETQq1 1 0.784314 rgBT /Ove metals (Li, Na and K). Applied Surface Science, 2016, 363, 197-208.	6.1	83
46	A DFT study on the formaldehyde (H 2 CO and (H 2 CO) 2) monitoring using pristine B 12 N 12 nanocluster. Physica E: Low-Dimensional Systems and Nanostructures, 2016, 78, 1-9.	2.7	25
47	Carbon monoxide monitoring using pristine and Cu-functionalized aluminum nitride and silicon carbide nanotubes; DFT study. Journal of Molecular Liquids, 2015, 204, 147-155.	4.9	5
48	A comparative theoretical study on the structural, electronic and nonlinear optical features of B12N12 and Al12N12 nanoclusters with the groups III, IV and V dopants. Superlattices and Microstructures, 2014, 76, 264-276.	3.1	57
49	A first principles study of pristine and Al-doped boron nitride nanotubes interacting with platinum-based anticancer drugs. Physica E: Low-Dimensional Systems and Nanostructures, 2014, 57, 47-55.	2.7	39
50	A theoretical study on pristine and doped germanium carbide nanoclusters. Journal of Materials Science: Materials in Electronics, 2014, 25, 4193-4199.	2.2	9
51	A Theoretical Study on the Influence of Carbon and Silicon Doping on the Structural and Electronic Properties of (BeO)12 Nanocluster. Journal of Inorganic and Organometallic Polymers and Materials, 2014, 24, 694-705.	3.7	15
52	A study on the influence of intramolecular O Hâ‹¯X (X = O and S) hydrogen bond formation on the aromaticity of heptafulvene derivatives, in which the methylene is replaced by <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" overflow="scroll"><mml:mrow><mml:msubsup><mml:mrow><mml:mtext>AlH</mml:mtext></mml:mrow><mml:mrow><mml:mn>2</m <mml:math xmlns:mml="http://www.w3.org. Computational and Theoretical Chemistry, 2014, 1039, 21-27.	2.5	2
53	The impact of intramolecular H-bonding on the aromatic character of substituted penta-fulvenes. Computational and Theoretical Chemistry, 2013, 1017, 31-36.	2.5	5
54	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.	7.8	42

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55	Formaldehyde adsorption on pristine, Al-doped and mono-vacancy defected boron nitride nanosheets: A first principles study. Computational Materials Science, 2012, 56, 122-130.	3.0	76
56	Evaluation of the Electrophilicites and Band Gaps of Conductive Polymers: A New Model. Macromolecular Theory and Simulations, 2012, 21, 529-534.	1.4	0
57	Shannon entropy as a new measure of aromaticity, Shannon aromaticity. Physical Chemistry Chemical Physics, 2010, 12, 4742.	2.8	153
58	Relative electrophilicity and aromaticity. Chemical Physics Letters, 2010, 484, 363-367.	2.6	10
59	Bond dissociation energies from a new electronegativity scale. Journal of Molecular Structure, 2009, 920, 110-113.	3.6	22
60	A New Scale of Electronegativity Based on Electrophilicity Index. Journal of Physical Chemistry A, 2008, 112, 3486-3491.	2.5	58
61	Endohedral M@B 40 (Mâ€‰=â€‰Na and Ca) metalloborospherenes as innovative potential carriers for chemotherapy melphalan drug: A theoretical study. Applied Organometallic Chemistry, 0, , e6411.	3.5	8