Sheida Ahmadi

List of Publications by Year in descending order

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SHEIDA ΔΗΜΑΟΙ

#	Article	IF	CITATIONS
1	Adsorption of toxic acrolein gas by Ag-decorated aluminum phosphide nanotubes. Solid State Communications, 2022, 343, 114657.	1.9	5
2	Study the Nature of the Interaction Between 5-Fluorouracil Anti-cancer Drug and Zinc Oxide Nanocage. Brazilian Journal of Physics, 2022, 52, 1.	1.4	3
3	Unraveling the effect of Ti doping on the sensing properties of AlN nanotubes toward acrylonitrile gas. Inorganic Chemistry Communication, 2022, 137, 109161.	3.9	5
4	Stereoselective cycloaddition of biologically active thioindoline with the smallest nanocage in gas phase versus solution via density functional theory. Journal of Physical Organic Chemistry, 2022, 35, .	1.9	0
5	A DFT quest for effects of fused rings on the stability of remote N-heterocyclic carbenes. Structural Chemistry, 2021, 32, 787-798.	2.0	8
6	Computational study of aÂB36 borophene as an electronic sensor for the anti-cancer drug cisplatinum. Journal of Computational Electronics, 2021, 20, 635-642.	2.5	11
7	Sensing properties of Al- and Si-doped HBC nanostructures toward Gamma-butyrolactone drug: A density functional theory study. Computational and Theoretical Chemistry, 2021, 1197, 113163.	2.5	9
8	A computational perspective of novel N â€heterocyclic silylenes using density functional theory. Journal of Physical Organic Chemistry, 2021, 34, e4197.	1.9	0
9	Characterization of IR spectroscopy, APT charge, ESP maps, and AIM analysis of C 20 and its C 20â€n Al n heterofullerene analogous (n = 1–5) using DFT. Journal of Physical Organic Chemistry, 2021, 34, e4198.	1.9	10
10	Thermodynamic stability, structural and electronic properties for the C20-nAln heterofullerenes (n = 1–5): a DFT study. Journal of Molecular Modeling, 2021, 27, 124.	1.8	13
11	Characterization of novel pyridineâ€derived <i>N</i> â€heterocyclic silylenes via density functional theory perspective. Journal of the Chinese Chemical Society, 2021, 68, 1405-1412.	1.4	8
12	A DFT study on the electronic detection of mercaptopurine drug by boron carbide nanosheets. Computational and Theoretical Chemistry, 2021, 1198, 113166.	2.5	26
13	Characterization of titanium influences on structure and thermodynamic stability of novel C20-nTin nanofullerenes (n=1–5): a density functional perspective. Journal of Molecular Modeling, 2021, 27, 176.	1.8	10
14	Kinetic stability and NBO analysis of the C20-nAln nanocages (nÂ=Â1–5) using DFT investigation. Journal of Molecular Structure, 2021, 1233, 130079.	3.6	8
15	Substituent effects on the stability of N â€heterocyclic germylenes using density functional theory. Journal of Physical Organic Chemistry, 2021, 34, e4266.	1.9	1
16	A density functional theory investigation on 1H-4-germapyridine-4-ylidene & the unsaturated heterocyclic substituted ones. Journal of Molecular Structure, 2021, 1238, 130427.	3.6	11
17	A DFT study on the Ag-decorated AlP nanosheets as chemical sensor for recognition of adrucil drug. Computational and Theoretical Chemistry, 2021, 1206, 113484.	2.5	5
18	A theoretical survey on the FCN detection by the intrinsic and Ti-doped boron carbide nanosheet. Computational and Theoretical Chemistry, 2021, 1206, 113490.	2.5	1

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19	Docking studies on an N ₄ -donor Schiff base ligand and its Cu(II) complex supported by structural, spectral and theoretical studies. Journal of Chemical Research, 2019, 43, 170-178.	1.3	3
20	Recent advances in the application of nano-catalysts for Hiyama cross-coupling reactions. RSC Advances, 2019, 9, 3185-3202.	3.6	38
21	A DFT study on nanocones, nanotubes (4,0), nanosheets and fullerene C ₆₀ as anodes in Mg-ion batteries. RSC Advances, 2019, 9, 853-862.	3.6	29
22	The effect of soft repulsive interactions on the diffusion of particles in quasi-one-dimensional channels: A hopping time approach. Journal of Chemical Physics, 2019, 150, 224501.	3.0	3
23	Odorless, convenient and one-pot synthesis of thioethers from organic halides and thiourea. Journal of Sulfur Chemistry, 2019, 40, 209-231.	2.0	13
24	Transition metal-catalyzed intramolecular cyclization of N-Boc-protected propargyl/ethynyl amines: a novel and convenient access to 2-oxazolidinone/oxazolone derivatives. Journal of the Iranian Chemical Society, 2019, 16, 617-627.	2.2	15
25	A walk around the decarboxylative C-S cross-coupling reactions. Journal of Sulfur Chemistry, 2019, 40, 88-112.	2.0	39
26	Protective effects of isatin and its synthetic derivatives against iron, copper and lead toxicity. Toxicology in Vitro, 2019, 54, 232-236.	2.4	9
27	A Facile and Promising Synthetic Strategy toward Functionalized 2 <i>H</i> -Chromenes from Aryl Propargyl Ethers. A Review. Organic Preparations and Procedures International, 2018, 50, 544-564.	1.3	3
28	Arylhydrazines: novel and versatile electrophilic partners in cross-coupling reactions. RSC Advances, 2018, 8, 33828-33844.	3.6	52
29	Cross-Dehydrogenative C–H/S–H Coupling Reactions. Topics in Current Chemistry, 2018, 376, 39.	5.8	72
30	Diaryl ethers synthesis: nano-catalysts in carbon-oxygen cross-coupling reactions. RSC Advances, 2018, 8, 19125-19143.	3.6	41
31	Decarboxylative cross-coupling reactions for P(O)–C bond formation. RSC Advances, 2018, 8, 26383-26398.	3.6	42
32	Three-component reaction of amines, epoxides, and carbon dioxide: A straightforward route to organic carbamates. Journal of CO2 Utilization, 2018, 27, 381-389.	6.8	53
33	Nano-structured Catalytic Systems in Cyanation of Aryl Halides with K4[Fe(CN)6]. Current Organic Chemistry, 2018, 22, 1862-1874.	1.6	6
34	Diffusion in quasi-one-dimensional channels: A small system n, p, T, transition state theory for hopping times. Journal of Chemical Physics, 2017, 146, 154505.	3.0	10
35	A new amino alcohol N _{py} N _{imine} N _{amine} O _{alcohol} -donor ligand: coordination toward zinc(II) and cadmium(II) halides and enantioselective products. Journal of Coordination Chemistry. 2017. 70. 3513-3522.	2.2	1