

Maryam Koohi

List of Publications by Year in descending order

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Version: 2024-02-01

30
papers

495
citations

623734

14
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794594

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all docs

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docs citations

30
times ranked

218
citing authors

#	ARTICLE	IF	CITATIONS
1	Visible light photocatalytic activity of reduced graphene oxide synergistically enhanced by successive inclusion of Fe_3O_4 , TiO_2 , and Ag nanoparticles. <i>Materials Science in Semiconductor Processing</i> , 2014, 26, 69-78.	4.0	31
2	Silicon impacts on structure, stability and aromaticity of $\text{C}_{20-n}\text{Si}_n$ heterofullerenes ($n=1-10$): A density functional perspective. <i>Journal of Molecular Structure</i> , 2017, 1127, 522-531.	3.6	31
3	Breathing viability into cyclonona-3,5,7-trienylidenes \pm -dimethyl and \pm -moieties at DFT. <i>Journal of Physical Organic Chemistry</i> , 2013, 26, 540-550.	1.9	26
4	2,2,9,9-tetramethylcyclonona-3,5,7-trienylidene vs its heterocyclic analogues: A quest for stable carbenes at DFT. <i>Journal of Physical Organic Chemistry</i> , 2013, 26, 908-916.	1.9	25
5	Substituent effects on cyclonona-3,5,7-trienylidenes: a quest for stable carbenes at density functional theory level. <i>Journal of Physical Organic Chemistry</i> , 2015, 28, 514-526.	1.9	25
6	Characterizations of B and N heteroatoms as substitutional doping on structure, stability, and aromaticity of novel heterofullerenes evolved from the smallest fullerene cage C_{20} : a density functional theory perspective. <i>Journal of Physical Organic Chemistry</i> , 2016, 29, 514-522.	1.9	25
7	Substituent effects on stability, MEP, NBO analysis, and reactivity of 2,2,9,9-tetrahalosilacyclonona-3,5,7-trienylidenes, at density functional theory. <i>Monatshefte für Chemie</i> , 2020, 151, 11-23.	1.8	23
8	Heteroatom impacts on structure, stability and aromaticity of $\text{X}_n\text{C}_{20-n}$ fullerenes: A theoretical prediction. <i>Computational and Theoretical Chemistry</i> , 2010, 940, 19-28.	1.5	21
9	Novel X- and Y-substituted heterofullerenes $\text{X}_4\text{Y}_4\text{C}_{12}$ developed from the nanocage C_{20} , where X = B, Al, Ga, Si and Y = N, P, As, Ge: a comparative investigation on their structural, stability, and electronic properties at DFT. <i>Structural Chemistry</i> , 2018, 29, 909-920.	2.0	21
10	A selective nanocatalyst for an efficient Ugi reaction: Magnetically recoverable $\text{Cu}(\text{acac})_2/\text{NH}_2\text{-Ti/SiO}_2@/\text{Fe}_3\text{O}_4$ nanoparticles. <i>Journal of Chemical Sciences</i> , 2013, 125, 1347-1357.	1.5	18
11	Cyclacenes and short zigzag nanotubes with alternating Ge-C bonds: theoretical impacts of Ge on the ground state, strain, and band gap. <i>Journal of Physical Organic Chemistry</i> , 2014, 27, 735-746.	1.9	18
12	Cyclonona-3,5,7-trienylidene and its Si, Ge, Sn, and Pb analogs versus their \pm -halogenated derivatives at B3LYP and MP2 methods. <i>Journal of Physical Organic Chemistry</i> , 2019, 32, e4013.	1.9	18
13	Substituent effect on structure, stability, and aromaticity of novel $\text{B}_n\text{N}_m\text{C}_{20-n-m}$ heterofullerenes. <i>Journal of Physical Organic Chemistry</i> , 2017, 30, e3682.	1.9	17
14	Structure, stability, and electronic properties of AlP nanocages evolved from the world's smallest caged fullerene C_{20} : A computational study at DFT. <i>Journal of Molecular Structure</i> , 2018, 1159, 118-134.	3.6	17
15	$\text{C}_{20-n}\text{Ge}_n$ heterofullerenes ($n=1-10$) on focus: a density functional perspective. <i>Monatshefte für Chemie</i> , 2015, 146, 1409-1417.	1.8	16
16	Characterization of nonsegregated C_{17}Si_3 heterofullerenic isomers using density functional theory method. <i>Journal of the Chinese Chemical Society</i> , 2018, 65, 1453-1464.	1.4	16
17	Substituted Hammick carbenes: The effects of fused rings and hetero atoms through DFT calculations. <i>Journal of Physical Organic Chemistry</i> , 2020, 33, e4023.	1.9	16
18	Characterization of C_{20} fullerene and its isolated $\text{C}_{20-n}\text{G}_n$ derivatives ($n=1-5$) by alternating germanium atom(s) in equatorial position: A DFT survey. <i>Heteroatom Chemistry</i> , 2018, 29, .		15

#	ARTICLE	IF	CITATIONS
19	Estimating the stability and reactivity of cyclic tetrahalo substituted germylenes: A density functional theory investigation. <i>Journal of Physical Organic Chemistry</i> , 2020, 33, e4032.	1.9	14
20	A density functional theory perspective on 2,2,9,9-tetrahalostannacyclonona-3,5,7-trienylidenes. <i>Journal of Physical Organic Chemistry</i> , 2020, 33, e4031.	1.9	14
21	Structure, stability, MEP, NICS, reactivity, and NBO of Si-Ge nanocages evolved from C ₂₀ fullerene at DFT. <i>Monatshefte für Chemie</i> , 2020, 151, 693-710.	1.8	14
22	A comparative study on the Ge ₆ C ₁₄ heterofullerene nanocages: a density functional survey. <i>Journal of Physical Organic Chemistry</i> , 2017, 30, e3678.	1.9	13
23	Transition state characteristics of planar singlet 2,4,6,8-cyclononatetraenylidenes and its halo derivatives, via ab initio. <i>Computational and Theoretical Chemistry</i> , 2005, 724, 61-71.	1.5	11
24	Mirror image conversions of cyclic conjugated non-planar allenes, C ₉ H ₇ X (X=H, F, Cl, Br). <i>Computational and Theoretical Chemistry</i> , 2005, 755, 91-98.	1.5	11
25	Ylide stabilized carbenes: a computational study. <i>Journal of Physical Organic Chemistry</i> , 2014, 27, 902-908.	1.9	11
26	Ring flips of allenes (C ₉ H ₇ X) over triplet carbenes at ab initio and DFT levels (X=H, F, Cl, Br). <i>Computational and Theoretical Chemistry</i> , 2007, 815, 21-29.	1.5	9
27	Umbrella inversions of cyclononatetraenylidenes at ab initio and DFT. <i>Computational and Theoretical Chemistry</i> , 2007, 810, 53-64.	1.5	8
28	Computational Study of Solvent Effects on Characterizations of (E)-3-X-Indoline-2-thiones Derivatives as Antivirus and Anticancer Compounds. <i>Bulletin of the Korean Chemical Society</i> , 2015, 36, 1985-1991.	1.9	4
29	(E)-3-X-Indoline-2-thiones as potent and selective inhibitors against different receptor tyrosine kinase (RTKs) in solution vs gas phase, at DFT. <i>Journal of Physical Organic Chemistry</i> , 2019, 32, e3929.	1.9	4
30	Introducing boranorcaradienes with more stability than their corresponding borepins: Reversal of tautomerization via substituents at theoretical levels. <i>Journal of Physical Organic Chemistry</i> , 2017, 30, e3714.	1.9	3