Reza Ghafouri

List of Publications by Year
in descending order

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52	345	840776 11	940533 16
papers	citations	h-index	g-index

52	52	52	221
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Mono- and multiply-functionalized fullerene derivatives through 1,3-dipolar cycloadditions: A DFT study. Physica E: Low-Dimensional Systems and Nanostructures, 2014, 56, 351-356.	2.7	32
2	A computational proof toward correlation between the theoretical chemical concept of electrophilicity index for the acceptors of C60 and C70 fullerene derivatives with the open-circuit voltage of polymer-fullerene solar cells. Solar Energy Materials and Solar Cells, 2012, 105, 125-131.	6.2	26
3	Exploring magnetic properties inside full equatorial BN-substituted fullerenes Cn (n=20, 24, 30, 36, 60,) Tj ETQq1 1 0.784314 rgBT /O 2012, 44, 1386-1391.	2.7	17
4	BN-Substituted fullerenes C60â^'2x (BN) x : a computational 11B and 15N NMR study. Structural Chemistry, 2012, 23, 1921-1929.	2.0	17
5	Functionalization of carbon ad-dimer defective single-walled carbon nanotubes through 1,3-dipolar cycloaddition: a DFT study. Structural Chemistry, 2015, 26, 507-515.	2.0	16
6	A computational investigation of 11B electric field gradient and chemical shielding tensors as well as NBO analysis in the B80 fullerene. Solid State Sciences, 2012, 14, 381-386.	3.2	15
7	A computational NICS and 13C NMR characterization of the polyfluorofullerenes C60Fn (n=18, 20, 24,) Tj ETQq1 1 0.784314 rgBT /O	1.7	13
8	A computational NICS and 13C NMR characterization of the substitution patterns of C70â^'2x(BN)x fullerenes (x=1â€“25). Journal of Physics and Chemistry of Solids, 2012, 73, 1378-1384.	4.0	12
9	1H and 29Si NMR investigation of SinHn polysilanes with nâ‰60: A DFT study. Physica E: Low-Dimensional Systems and Nanostructures, 2012, 44, 2099-2104.	2.7	12
10	Silicon doping of defect sites in Stoneâ€“Wales defective carbon nanotubes: A density functional theory study. Superlattices and Microstructures, 2013, 60, 1-9.	3.1	11
11	An investigation of curvature effects on the nitrogen and boron chemical shielding tensors as well as NICS characterization of BN nanotubes with Stoneâ€“Wales defects: A DFT study. Superlattices and Microstructures, 2013, 55, 33-44.	3.1	11
12	A computational investigation of the electronic properties of Octahedral Al n N n and Al n P n cages (nÂ=Â12, 16, 28, 36, and 48). Structural Chemistry, 2013, 24, 681-689.	2.0	11
13	1,3-Dipolar cycloaddition of BC2N nanotubes: A DFT study. Computational and Theoretical Chemistry, 2014, 1034, 32-37.	2.5	11
14	Exploring electronic structures for the most stable isomers of C12B6N6 and B6N6C12 heterofullerenes based on NMR, NICS and NBO analysis: A DFT study. Physica E: Low-Dimensional Systems and Nanostructures, 2012, 44, 1992-1998.	2.7	10
15	A Computational NICS and 13C NMR Characterization of C60â^'n Si n Heterofullerenes (nÂ=Â1, 2, 6, 12, 20,) Tj ETQq1 1 0.784314 rg	3.3	9
16	Functionalization of pentagonâ€“pentagon edges of fullerenes by cyclic polysulfides: A DFT study. Journal of Physics and Chemistry of Solids, 2016, 92, 26-31.	4.0	9
17	Density functional investigation of the electronic properties of B80 fullerene exposed to regioselective chemisorption of nucleophiles NH3, PH3 and AsH3. Superlattices and Microstructures, 2012, 52, 861-871.	3.1	8
18	Carbon Doping of Defect Sites in Stoneâ€“Wales Defective Boron-nitride Nanotubes: A Density Functional Theory Study. Journal of Cluster Science, 2013, 24, 865-879.	3.3	7

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19	(SiH)48X12 Heterofullerenes with the Group III and V Dopants: A DFT Prediction of Geometry, Stability, and Electronic Structure. Journal of Cluster Science, 2014, 25, 505-515.	3.3	7
20	Exploring the electronic and magnetic properties of C60 fullerene dimers with ladderane-like hexagonal bridges. Computational and Theoretical Chemistry, 2012, 1000, 85-91.	2.5	6
21	Investigation of curvature effects on the nitrogen and boron electric field gradient and chemical shielding tensors in the mono-BN-substituted fullerenes: A density functional theory. Physica E: Low-Dimensional Systems and Nanostructures, 2012, 45, 183-189.	2.7	6
22	Exploring magnetic properties and Curved Ï€-Conjugation of BxNyCz nanotubes using density functional theory. Superlattices and Microstructures, 2013, 57, 66-76.	3.1	6
23	Stoneâ€“Wales defect formation in the zigzag and armchair BC2N nanotubes: A DFT study. Physica E: Low-Dimensional Systems and Nanostructures, 2014, 58, 94-100.	2.7	6
24	A computational investigation of electronic structure as well as 19F and 29Si chemical shielding tensors in the fluorinated silicon fullerenes SinFn (nâ‰60). Physica E: Low-Dimensional Systems and Nanostructures, 2013, 48, 13-20.	2.7	5
25	Exploring pentagon-heptagon pair defects in the triangular graphene quantum dots: A computational study. Materials Chemistry and Physics, 2016, 175, 223-232.	4.0	5
26	Theoretical studies on one-dimensional polymers constructed from BN-substituted C36 fullerene. Computational and Theoretical Chemistry, 2013, 1017, 1-6.	2.5	4
27	Evaluation of on-cage phosphorus doping of hydrogenated silicon fullerenes: a computational study. Structural Chemistry, 2014, 25, 37-42.	2.0	4
28	Boron-nitride ad-unit and carbon ad-dimer defects in the boron nitride nanotubes. Journal of Physics and Chemistry of Solids, 2015, 79, 7-13.	4.0	4
29	A computational investigation of 11B and 15N chemical shielding tensors as well as local aromaticity based on NICS characterization in the N/B doped triangular graphene quantum dots. Superlattices and Microstructures, 2013, 62, 207-216.	3.1	3
30	Exploring Electronic Properties of Si_{20-n}H_{20-n}P_nHeterofullerenes (N= 1,) Tj ETQq0 0 0 rgBT /Overlock Related Elements, 2014, 189, 60-73.	1.6	3
31	Theoretical Investigation of Mono and Multiply Oxygenated C70 Fullerenes. Journal of Cluster Science, 2014, 25, 1109-1119.	3.3	3
32	Fully and partially exohydrogenated Si80 fullerene cage: a DFT study. Structural Chemistry, 2014, 25, 575-581.	2.0	3
33	Theoretical identification of the lowest energy structure of C70â^'n Si n , nÂ=Â1, 2, 6, 10, and 20 heterofullerenes. Structural Chemistry, 2014, 25, 617-623.	2.0	3
34	Exploring the electronic and magnetic properties of zigzag and armchair BC2N nanotubes: a DFT study. Structural Chemistry, 2014, 25, 95-102.	2.0	3
35	1,3-Dipolar Cycloaddition in Stoneâ€“Wales Defective Carbon Nanotubes: A Computational Study. Journal of Cluster Science, 2015, 26, 581-594.	3.3	3
36	Exploring the Mechanism of Reactions of SiX3 and CX3 Radicals with Si20X20 Fullerenes (XÂ=ÂH, F): A Density Functional Study. Journal of Cluster Science, 2016, 27, 1719-1728.	3.3	3

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37	COMPUTATIONAL NICS AND ¹³C NMR ChARACTERIZATION OF SUBSTITUTION PATTERNS OF C_{60-n}N_n FULLERENES (n = 1â€“12). Journal of Theoretical and Computational Chemistry, 2013, 12, 1350009.	1.8	2
38	Electronic and Chemical Characterization of Aluminumâ€“Nitrogen (AlN) Substituted Fullerenes: C58AlN to C24Al12N12. Journal of Cluster Science, 2013, 24, 327-339.	3.3	2
39	BN Belts: From Small Fullerenes to Nanocapsules. Journal of Cluster Science, 2014, 25, 1173-1185.	3.3	2
40	A Computational Investigation of the Electronic Properties of Partially Hydrogenated Fullerenes C₆₀H_n(n= 18, 20, 24, 36 and 48). Fullerenes Nanotubes and Carbon Nanostructures, 2015, 23, 40-48.	2.1	2
41	Characterization of Hydrogen Bonds in the End-Functionalized Single-Wall Carbon Nanotubes: A DFT Study. Nano, 2015, 10, 1550036.	1.0	2
42	Exploring 11B and 15N NMR parameters of C70â^'2x (BN) x fullerenes (xÂ=Â3â€“25) in connection with local structures and curvature effects: a DFT study. Monatshefte FÃ¼r Chemie, 2014, 145, 411-419.	1.8	1
43	X24Y24 fullerene-like cages with the group III and V elements XÂ=ÂB, Al, and Ga; YÂ=ÂN, P, and As: a DFT prediction. Monatshefte FÃ¼r Chemie, 2015, 146, 1241-1247.	1.8	1
44	Exploring the simultaneous existence of Stone-Wales and carbon ad-dimer defects in the zigzag single-walled carbon nanotubes. Physica E: Low-Dimensional Systems and Nanostructures, 2016, 83, 238-245.	2.7	1
45	Theoretical study on the mono and multiply oxygenated Si₆₀H₆₀ fullerene. Molecular Physics, 2016, 114, 819-828.	1.7	1
46	AlSi2P nanotubes: a theoretical study. Structural Chemistry, 2016, 27, 525-533.	2.0	1
47	Computational study for the circular redox reaction of N2O with CO catalyzed by fullerometallic cations C60Fe+ and C70Fe+. Journal of Molecular Graphics and Modelling, 2017, 72, 50-57.	2.4	1
48	Chlorofluorofullerenes (CFFs). Structural Chemistry, 2017, 28, 1707-1716.	2.0	1
49	Theoretical study on the mechanism of reactions of CX3 radicals (XÂ=ÂH, F, Cl and Br) with C20H20 and C20F20 fullerenes. Journal of Molecular Structure, 2017, 1127, 296-302.	3.6	1
50	Hydrogen-abstraction reactions of fully hydrogenated silicon fullerene cages with the amino radical: a density functional study. Structural Chemistry, 2018, 29, 607-614.	2.0	1
51	Polarizability of the Si60H60 Derivatives Containing Epoxide Moieties (Si60H60â^'2nOn with n up to 30): A DFT Study. Journal of Cluster Science, 2018, 29, 889-896.	3.3	1
52	Exploring Adjacent Pentagons in Non-IPR and SW Defective Si60 and Si70 Silicon Fullerenes: a Computational Study. Silicon, 2019, 11, 323-329.	3.3	1