Meysam Najafi

List of Publications by Year
in descending order

41 papers	191 citations	7 h-index	12 g-index
47 all docs	47 docs citations	47 times ranked	202 citing authors

1307594

1199594

#	ARTICLE	IF	CITATIONS
1	A theoretical investigation on the potential of copper- and zinc-doped nanotubes as catalysts for the oxidation of SO2 (SO2â€‰+â€‰Â½O2â€‰â†’â€‰SO3) and CO (COâ€‰+â€‰Â½O2â€‰â†’â€‰CO2). Journal of Computationa 19, 55-61.	2.5	1
2	DFT prediction of oxygen reduction reaction on B-SiNT catalyst in fuel cells. Journal of Electroanalytical Chemistry, 2020, 858, 113814.	3.8	0
3	Possibility of NiO, ZrO2, ZnO and GrO2 Attached to Silicon and Carbon Nanostructures as Anode of Battery: Computational Examination. Silicon, 2020, 12, 2107-2110.	3.3	5
4	Zinc oxide and germanium dioxide adsorbed on silicon nanocage as anodes in lithium-ion battery and potassium-ion battery. Ionics, 2020, 26, 2211-2215.	2.4	4
5	Aluminum Doped Silicon Nanocage as High Efficiency Catalysts to Oxygen Reduction Reaction. Russian Journal of Electrochemistry, 2020, 56, 775-780.	0.9	1
6	Investigation of Potential of Oxygen Reduction Reaction at Aluminum Doped Carbon Nanocage (Al-C72) as a Catalyst. Russian Journal of Physical Chemistry B, 2020, 14, 40-44.	1.3	4
7	A DFT investigation of performance of metal-doped nanotubes as acceptable catalysts to SiO oxidation. Bulletin of Materials Science, 2020, 43, 1.	1.7	0
8	Aluminum-doped silicon nanocage and boron-doped carbon nanocage as catalysts to oxygen reduction reaction (ORR): a computational investigation. Ionics, 2020, 26, 3085-3090.	2.4	4
9	Theoretical investigation of oxygen reduction process on the Si nanocone (Al-SiNC) as efficiency catalyst in fuel cells. Journal of Molecular Liquids, 2020, 303, 112662.	4.9	1
10	Investigation of potentials of $$hbox {C}_{30}$$ and $$hbox {Ge}_{30}$$ as anode in metal-ion batteries. Bulletin of Materials Science, 2020, 43, 1.	1.7	0
11	Theoretical examination of oxygen reduction reaction (ORR) on carbon nanocone (CNC) for fuel cells. Bulletin of Materials Science, 2020, 43, 1.	1.7	1
12	Titanium-doped carbon and boron nitride nanocages (Tiâ€“$$hbox {C}_{48}$$ and Tiâ€“$$hbox) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 {ClO}_{2}$$ reaction: theoretical study. Bulletin of Materials Science, 2020, 43, 1.	1.7	1
13	Oxidation of Methylene via Sn-adsorbed Boron Nitride Nanocage (B30N30): DFT Investigation. Silicon, 2019, 11, 995-1000.	3.3	0
14	Potential of Ge-adopted Boron Nitride Nanotube as Catalyst for Sulfur Dioxide Oxidation. Protection of Metals and Physical Chemistry of Surfaces, 2019, 55, 671-676.	1.1	24
15	Investigation of performance of aluminum doped carbon nanotube (8, 0) as adequate catalyst to oxygen reduction reaction. Journal of Molecular Graphics and Modelling, 2019, 92, 123-130.	2.4	3
16	Examination of potential of B-CNT (6, 0), Al-CNT (6, 0) and Ga-CNT (6, 0) as novel catalysts to oxygen reduction reaction: A DFT study. Journal of Molecular Liquids, 2019, 290, 111366.	4.9	4
17	Titanium oxide (TiO) and Ruthenium dioxide (RuO2) attached to silicon nanotube (7,â€¯0) as electrodes of lithium-, sodium- and potassium-ion batteries: Computational investigation. Tetrahedron Letters, 2019, 60, 150933.	1.4	1
18	Role of boron doped silicon nanocage (B-Si48) as catalyst for oxygen reduction reaction in fuel cells. Chemical Physics Letters, 2019, 731, 136629.	2.6	5

#	Article	IF	Citations
19	Potential of cobalt-doped nanocages (Coâ€“B36N36 and Coâ€“C72) for SO oxidation (SOâ€‰+â€‰Â½ O2â€‰â†’â€‰SO2): computational investigation. Monatshefte FÃ¼r Chemie, 2019, 150, 1779-1784.	1.8	3
20	Theoretical investigation of oxidation of NO (NOÂ+ Â½ O2 â†’ NO2) on surfaces of nickel-doped nanocages (Niâ€“C60 and Niâ€“B30N30). Journal of Molecular Graphics and Modelling, 2019, 91, 140-147.	2.4	1
21	Potential of Carbon, Silicon, Boron Nitride and Aluminum Phosphide Nanocages as Anodes of Lithium, Sodium and Potassium Ion Batteries: A DFT Study. Russian Journal of Physical Chemistry B, 2019, 13, 156-164.	1.3	7
22	Adsorbed CdO, TiO, RuO2, and IrO2 to silicon nanotube and carbon nanocage for anode of metal-ion battery: a computational study. Monatshefte FÃ¼r Chemie, 2019, 150, 2025-2028.	1.8	3
23	Theoretical investigation of the ORR on boronâ€“silicon nanotubes (Bâ€“SiNTs) as acceptable catalysts in fuel cells. RSC Advances, 2019, 9, 31572-31582.	3.6	4
24	Potential of Si14Ge14 and B14P14 nanocages as electrodes of metal-ion batteries: a theoretical investigation. Journal of Solid State Electrochemistry, 2019, 23, 759-769.	2.5	3
25	$$hbox {C}_{32}hbox {, Si}_{32}$$ C 32 , Si 32 and $$hbox {B}_{16}hbox {N}_{. Bulletin of Materials Science, 2019, 42, 1.	1.7	0
26	Potential of Doped Nanocones as Catalysts for N2Oâ€‰+â€‰CO Reaction: Theoretical Investigation. Journal of Cluster Science, 2019, 30, 61-67.	3.3	3
27	Theoretical investigation of the use of nanocages with an adsorbed halogen atom as anode materials in metal-ion batteries. Journal of Molecular Modeling, 2018, 24, 64.	1.8	4
28	DFT Investigation of the Potential of B21N21 and Al21P21 Nanocages as Anode Electrodes in Metal Ion Batteries. Journal of Cluster Science, 2018, 29, 879-887.	3.3	3
29	DFT study of cyanide oxidation on surface of Ge-embedded carbon nanotube. Chemical Physics Letters, 2018, 695, 44-50.	2.6	7
30	A Theoretical Examination of the Antioxidant Activity of NH2, OMe, and tert-Butyl Sesamol Derivatives and Their Drug Delivery with C60 Nanocage. Russian Journal of Physical Chemistry A, 2018, 92, 2757-2760.	0.6	1
31	Sn-adopted fullerene $$(hbox {C}_{60})$$ (C 60) nanocage as acceptable catalyst for silicon monoxide oxidation. Bulletin of Materials Science, 2018, 41, 1.	1.7	1
32	F, Cl, Br Doped Ge44 and Al22P22 Nanocages As Anode Electrode Materials of Li, Na, and K ion Batteries. Russian Journal of Physical Chemistry A, 2018, 92, 2282-2288.	0.6	1
33	Possibility of C38 and Si19Ge19 Nanocages in Anode of Metal Ion Batteries: Computational Examination. Acta Chimica Slovenica, 2018, 65, 303-311.	0.6	26
34	Theoretical investigation of properties of boron nitride nanocages and nanotubes as high-performance anode materials for lithium-ion batteries. Canadian Journal of Chemistry, 2017, 95, 687-690.	1.1	10
35	Antioxidant activity of omega-3 derivatives and their delivery via nanocages and nanocones: DFT and experimental in vivo investigation. Journal of Molecular Modeling, 2017, 23, 326.	1.8	8
36	Theoretical and Experimental in vivo Study of Antioxidant Activity of Crocin in Order to Propose Novel Derivatives with Higher Antioxidant Activity and Their Delivery via Nanotubes and Nanocones. Inflammation, 2017, 40, 1794-1802.	3.8	8

#	Article	IF	Citations
37	A theoretical investigation of the N2O + SO2 reaction on surfaces of P-doped C60 nanocage and Si-doped B30N30 nanocage. Results in Physics, 2017, 7, 2619-2625.	4.1	4
38	A theoretical study of adsorption of tyrosol derivatives as antioxidant drugs on the boron nitride (BN)-nanotube (9, 0) surface. International Journal of Food Properties, 2017, , 1-9.	3.0	0
39	Adsorption of carbon dioxide (CO2) at S functionalized boron nitride (BN) and aluminum nitride (AlN) nanotubes (9, 0): A quantum chemical investigation. Applied Surface Science, 2016, 384, 380-385.	6.1	8
40	On the antioxidant activity of ortho- and meta-substituted indolin-2-one derivatives. Monatshefte FÃ¼r Chemie, 2014, 145, 291-299.	1.8	10
41	DFT/B3LYP Study of the Substituent Effects on the Reaction Enthalpies of the Antioxidant Mechanisms of Sesamol Derivatives in the Gas phase and water. Canadian Journal of Chemistry, 2012, 90, 915-926.	1.1	12