

# Meysam Najafi

## List of Publications by Year in descending order

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Version: 2024-02-01

41  
papers

191  
citations

1307594

7  
h-index

1199594

12  
g-index

47  
all docs

47  
docs citations

47  
times ranked

202  
citing authors

#	ARTICLE	IF	CITATIONS
1	Possibility of C <sub>38</sub> and Si <sub>19</sub> Ge <sub>19</sub> Nanocages in Anode of Metal Ion Batteries: Computational Examination. <i>Acta Chimica Slovenica</i> , 2018, 65, 303-311.	0.6	26
2	Potential of Ge-adopted Boron Nitride Nanotube as Catalyst for Sulfur Dioxide Oxidation. <i>Protection of Metals and Physical Chemistry of Surfaces</i> , 2019, 55, 671-676.	1.1	24
3	DFT/B3LYP Study of the Substituent Effects on the Reaction Enthalpies of the Antioxidant Mechanisms of Sesamol Derivatives in the Gas phase and water. <i>Canadian Journal of Chemistry</i> , 2012, 90, 915-926.	1.1	12
4	On the antioxidant activity of ortho- and meta-substituted indolin-2-one derivatives. <i>Monatshefte für Chemie</i> , 2014, 145, 291-299.	1.8	10
5	Theoretical investigation of properties of boron nitride nanocages and nanotubes as high-performance anode materials for lithium-ion batteries. <i>Canadian Journal of Chemistry</i> , 2017, 95, 687-690.	1.1	10
6	Adsorption of carbon dioxide (CO <sub>2</sub> ) at S functionalized boron nitride (BN) and aluminum nitride (AlN) nanotubes (9, 0): A quantum chemical investigation. <i>Applied Surface Science</i> , 2016, 384, 380-385.	6.1	8
7	Antioxidant activity of omega-3 derivatives and their delivery via nanocages and nanocones: DFT and experimental in vivo investigation. <i>Journal of Molecular Modeling</i> , 2017, 23, 326.	1.8	8
8	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. <i>Inflammation</i> , 2017, 40, 1794-1802.	3.8	8
9	DFT study of cyanide oxidation on surface of Ge-embedded carbon nanotube. <i>Chemical Physics Letters</i> , 2018, 695, 44-50.	2.6	7
10	Potential of Carbon, Silicon, Boron Nitride and Aluminum Phosphide Nanocages as Anodes of Lithium, Sodium and Potassium Ion Batteries: A DFT Study. <i>Russian Journal of Physical Chemistry B</i> , 2019, 13, 156-164.	1.3	7
11	Role of boron doped silicon nanocage (B-Si <sub>48</sub> ) as catalyst for oxygen reduction reaction in fuel cells. <i>Chemical Physics Letters</i> , 2019, 731, 136629.	2.6	5
12	Possibility of NiO, ZrO <sub>2</sub> , ZnO and GrO <sub>2</sub> Attached to Silicon and Carbon Nanostructures as Anode of Battery: Computational Examination. <i>Silicon</i> , 2020, 12, 2107-2110.	3.3	5
13	A theoretical investigation of the N <sub>2</sub> O + SO <sub>2</sub> reaction on surfaces of P-doped C <sub>60</sub> nanocage and Si-doped B <sub>30</sub> N <sub>30</sub> nanocage. <i>Results in Physics</i> , 2017, 7, 2619-2625.	4.1	4
14	Theoretical investigation of the use of nanocages with an adsorbed halogen atom as anode materials in metal-ion batteries. <i>Journal of Molecular Modeling</i> , 2018, 24, 64.	1.8	4
15	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. <i>Journal of Molecular Liquids</i> , 2019, 290, 111366.	4.9	4
16	Theoretical investigation of the ORR on boron-silicon nanotubes (B-SiNTs) as acceptable catalysts in fuel cells. <i>RSC Advances</i> , 2019, 9, 31572-31582.	3.6	4
17	Zinc oxide and germanium dioxide adsorbed on silicon nanocage as anodes in lithium-ion battery and potassium-ion battery. <i>Ionics</i> , 2020, 26, 2211-2215.	2.4	4
18	Investigation of Potential of Oxygen Reduction Reaction at Aluminum Doped Carbon Nanocage (Al-C <sub>72</sub> ) as a Catalyst. <i>Russian Journal of Physical Chemistry B</i> , 2020, 14, 40-44.	1.3	4

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19	Aluminum-doped silicon nanocage and boron-doped carbon nanocage as catalysts to oxygen reduction reaction (ORR): a computational investigation. <i>Ionics</i> , 2020, 26, 3085-3090.	2.4	4
20	DFT Investigation of the Potential of B <sub>21</sub> N <sub>21</sub> and Al <sub>21</sub> P <sub>21</sub> Nanocages as Anode Electrodes in Metal Ion Batteries. <i>Journal of Cluster Science</i> , 2018, 29, 879-887.	3.3	3
21	Investigation of performance of aluminum doped carbon nanotube (8, 0) as adequate catalyst to oxygen reduction reaction. <i>Journal of Molecular Graphics and Modelling</i> , 2019, 92, 123-130.	2.4	3
22	Potential of cobalt-doped nanocages (Co@B <sub>36</sub> N <sub>36</sub> and Co@C <sub>72</sub> ) for SO oxidation (SO + 1/2 O <sub>2</sub> → SO <sub>2</sub> ): computational investigation. <i>Monatshefte für Chemie</i> , 2019, 150, 1779-1784.	1.8	3
23	Adsorbed CdO, TiO, RuO <sub>2</sub> , and IrO <sub>2</sub> to silicon nanotube and carbon nanocage for anode of metal-ion battery: a computational study. <i>Monatshefte für Chemie</i> , 2019, 150, 2025-2028.	1.8	3
24	Potential of Si <sub>14</sub> Ge <sub>14</sub> and B <sub>14</sub> P <sub>14</sub> nanocages as electrodes of metal-ion batteries: a theoretical investigation. <i>Journal of Solid State Electrochemistry</i> , 2019, 23, 759-769.	2.5	3
25	Potential of Doped Nanocones as Catalysts for N <sub>2</sub> O + CO Reaction: Theoretical Investigation. <i>Journal of Cluster Science</i> , 2019, 30, 61-67.	3.3	3
26	A Theoretical Examination of the Antioxidant Activity of NH <sub>2</sub> , OMe, and tert-Butyl Sesamol Derivatives and Their Drug Delivery with C <sub>60</sub> Nanocage. <i>Russian Journal of Physical Chemistry A</i> , 2018, 92, 2757-2760.	0.6	1
27	Sn-adopted fullerene C <sub>60</sub> nanocage as acceptable catalyst for silicon monoxide oxidation. <i>Bulletin of Materials Science</i> , 2018, 41, 1.	1.7	1
28	F, Cl, Br Doped Ge <sub>44</sub> and Al <sub>22</sub> P <sub>22</sub> Nanocages As Anode Electrode Materials of Li, Na, and K ion Batteries. <i>Russian Journal of Physical Chemistry A</i> , 2018, 92, 2282-2288.	0.6	1
29	Titanium oxide (TiO) and Ruthenium dioxide (RuO <sub>2</sub> ) attached to silicon nanotube (7,0) as electrodes of lithium-, sodium- and potassium-ion batteries: Computational investigation. <i>Tetrahedron Letters</i> , 2019, 60, 150933.	1.4	1
30	Theoretical investigation of oxidation of NO (NO + 1/2 O <sub>2</sub> → NO <sub>2</sub> ) on surfaces of nickel-doped nanocages (Ni@C <sub>60</sub> and Ni@B <sub>30</sub> N <sub>30</sub> ). <i>Journal of Molecular Graphics and Modelling</i> , 2019, 91, 140-147.	2.4	1
31	A theoretical investigation on the potential of copper- and zinc-doped nanotubes as catalysts for the oxidation of SO <sub>2</sub> (SO <sub>2</sub> + 1/2 O <sub>2</sub> → SO <sub>3</sub> ) and CO (CO + 1/2 O <sub>2</sub> → CO <sub>2</sub> ). <i>Journal of Computational Chemistry</i> , 2019, 40, 55-61.	1.7	1
32	Aluminum Doped Silicon Nanocage as High Efficiency Catalysts to Oxygen Reduction Reaction. <i>Russian Journal of Electrochemistry</i> , 2020, 56, 775-780.	0.9	1
33	Theoretical investigation of oxygen reduction process on the Si nanocone (Al-SiNC) as efficiency catalyst in fuel cells. <i>Journal of Molecular Liquids</i> , 2020, 303, 112662.	4.9	1
34	Theoretical examination of oxygen reduction reaction (ORR) on carbon nanocone (CNC) for fuel cells. <i>Bulletin of Materials Science</i> , 2020, 43, 1.	1.7	1
35	Titanium-doped carbon and boron nitride nanocages (Ti@C <sub>48</sub> and Ti@Tj ETQq1 1 0.784314 rgBT /Overlook {ClO}_{2}) reaction: theoretical study. <i>Bulletin of Materials Science</i> , 2020, 43, 1.	1.7	1
36	A theoretical study of adsorption of tyrosol derivatives as antioxidant drugs on the boron nitride (BN)-nanotube (9, 0) surface. <i>International Journal of Food Properties</i> , 2017, , 1-9.	3.0	0

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37	Oxidation of Methylene via Sn-adsorbed Boron Nitride Nanocage (B30N30): DFT Investigation. Silicon, 2019, 11, 995-1000.	3.3	0
38	$\text{C}_{32}$ , Si <sub>32</sub> and $\text{B}_{16}\text{N}_4$ . Bulletin of Materials Science, 2019, 42, 1.	1.7	0
39	DFT prediction of oxygen reduction reaction on B-SiNT catalyst in fuel cells. Journal of Electroanalytical Chemistry, 2020, 858, 113814.	3.8	0
40	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
41	Investigation of potentials of $\text{C}_{30}$ and $\text{Ge}_{30}$ as anode in metal-ion batteries. Bulletin of Materials Science, 2020, 43, 1.	1.7	0