Diego Guedes-Sobrinho

List of Publications by Year
in descending order

18	386	840776 11	888059 17
papers	citations	h-index	g-index

18	18	18	466
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Theoretical Study of the Structural, Energetic, and Electronic Properties of 55-Atom Metal Nanoclusters: A DFT Investigation within van der Waals Corrections, Spinâ€“Orbit Coupling, and PBE+U of 42 Metal Systems. Journal of Physical Chemistry C, 2016, 120, 28844-28856.	3.1	75
2	Structure, Electronic, and Magnetic Properties of Binary Pt_nTM_{55â€“n} (TM = Fe, Co, Ni, Cu, Zn) Nanoclusters: A Density Functional Theory Investigation. Journal of Physical Chemistry C, 2015, 119, 15669-15679.	3.1	66
3	Comparison of the Performance of van der Waals Dispersion Functionals in the Description of Water and Ethanol on Transition Metal Surfaces. Journal of Physical Chemistry C, 2018, 122, 1577-1588.	3.1	36
4	Theoretical Investigation of the Adsorption Properties of CO, NO, and OH on Monometallic and Bimetallic 13-Atom Clusters: The Example of Cu₁₃, Pt₇Cu₆, and Pt₁₃. Journal of Physical Chemistry A, 2015, 119, 11565-11573.	2.5	32
5	Nanocrystals self-assembled in superlattices directed by the solventâ€“organic capping interaction. Nanoscale, 2013, 5, 5602-5610.	5.6	28
6	Physical and Chemical Properties of Unsupported (MO₂)_n Clusters for M = Ti, Zr, or Ce and n = 1â€“15: A Density Functional Theory Study Combined with the Tree-Growth Scheme and Euclidean Similarity Distance Algorithm. Journal of Physical Chemistry C, 2018, 122, 27702-27712.	3.1	25
7	Ab Initio Investigation of Atomistic Insights into the Nanoflake Formation of Transition-Metal Dichalcogenides: The Examples of MoS₂, MoSe₂, and MoTe₂. Journal of Physical Chemistry C, 2018, 122, 27059-27069.	3.1	24
8	Relativistic DFT-1/2 Calculations Combined with a Statistical Approach for Electronic and Optical Properties of Mixed Metal Hybrid Perovskites. Journal of Physical Chemistry Letters, 2019, 10, 4245-4251.	4.6	20
9	Size-Induced Phase Evolution of MoSe₂ Nanoflakes Revealed by Density Functional Theory. Journal of Physical Chemistry C, 2018, 122, 20483-20488.	3.1	17
10	Thermodynamic Stability and Structural Insights for CH3NH3Pb1â^'xSixI3, CH3NH3Pb1â^'xGexI3, and CH3NH3Pb1â^'xSnxI3 Hybrid Perovskite Alloys: A Statistical Approach from First Principles Calculations. Scientific Reports, 2019, 9, 11061.	3.3	14
11	Ab Initio Investigation of the Role of CO Adsorption on the Physical Properties of 55-Atom PtCo Nanoalloys. Journal of Physical Chemistry C, 2017, 121, 27721-27732.	3.1	12
12	Density functional investigation of the adsorption effects of PH3 and SH2 on the structure stability of the Au55 and Pt55 nanoclusters. Journal of Chemical Physics, 2017, 146, 164304.	3.0	9
13	Bulk Rashba Effect Splitting and Suppression in Polymorphs of Metal Iodine Perovskites. Journal of Physical Chemistry Letters, 2021, 12, 7245-7251.	4.6	9
14	(Meta-)stability and Coreâ€“Shell Dynamics of Gold Nanoclusters at Finite Temperature. Journal of Physical Chemistry Letters, 2019, 10, 685-692.	4.6	8
15	Assessment of the van der Waals, Hubbard U parameter and <scp>spinâ€orbit</scp> coupling corrections on the <scp>2D</scp>/<scp>3D</scp> structures from metal gold congeners clusters. Journal of Computational Chemistry, 2022, 43, 230-243.	3.3	4
16	Impact of the Polymorphism and Relativistic Effects on the Electronic Properties of Inorganic Metal Halide Perovskites. Journal of Physical Chemistry C, 2022, 126, 2131-2140.	3.1	4
17	Influence of electrosynthesis methods in the electrocatalytical and morphological properties of cobalt and nickel hexacyanoferrate films. Electrochimica Acta, 2020, 361, 137021.	5.2	2
18	The effect of different energy portions on the 2D/3D stability swapping for 13-atom metal clusters. Physical Chemistry Chemical Physics, 2022, 24, 6515-6524.	2.8	1