Maurcio Jeomar Piotrowski

List of Publications by Year in Descending Order

42 papers	953 citations	17 h-index	30 g-index
46 ext. papers	1,153 ext. citations	3.6 avg, IF	4.59 L-index

#	Paper	IF	Citations
42	Electrochemical, theoretical, and analytical investigation of the phenylurea herbicide fluometuron at a glassy carbon electrode. *Electrochimica Acta*, **2022**, 408, 139945	6.7	0
41	Stability Changes in Iridium Nanoclusters via Monoxide Adsorption: A DFT Study within the van der Waals Corrections. *Journal of Physical Chemistry A*, **2021**, 125, 4805-4818	2.8	1
40	Energy Decomposition to Access the Stability Changes Induced by CO Adsorption on Transition-Metal 13-Atom Clusters. *Journal of Chemical Information and Modeling*, **2021**, 61, 2294-2301	6.1	2
39	The design of anion-π interactions and hydrogen bonds for the recognition of chloride, bromide and nitrate anions. *Physical Chemistry Chemical Physics*, **2021**, 23, 11455-11465	3.6	1
38	Designing boron and metal complexes for fluoride recognition: a computational perspective. *Physical Chemistry Chemical Physics*, **2021**, 23, 22768-22778	3.6	
37	Tracking the role of trans-ligands in ruthenium–NO bond lability: computational insight. *New Journal of Chemistry*, **2020**, 44, 11448-11456	3.6	2
36	The anionic recognition mechanism based on polyol and boronic acid receptors. *New Journal of Chemistry*, **2020**, 44, 5564-5571	3.6	1
35	Structural and Electronic Properties of Bulk ZnX (X = O, S, Se, Te), ZnF, and ZnO/ZnF: A DFT Investigation within PBE, PBE + , and Hybrid HSE Functionals. *Journal of Physical Chemistry A*, **2020**, 124, 3778-3785	2.8	17
34	Investigation of CO Adsorption on 13-Atom 4d Clusters. *Journal of Chemical Information and Modeling*, **2020**, 60, 537-545	6.1	11
33	How does the acidic milieu interfere in the capability of ruthenium nitrosyl complexes to release nitric oxide?. *New Journal of Chemistry*, **2020**, 44, 773-779	3.6	4
32	A theoretical indicator of transition-metal nanoclusters applied in the carbon nanotube nucleation process: a DFT study. *Dalton Transactions*, **2020**, 49, 492-503	4.3	6
31	Ab Initio Insights into the Formation Mechanisms of 55-Atom Pt-Based Core–Shell Nanoalloys. *Journal of Physical Chemistry C*, **2020**, 124, 1158-1164	3.8	11
30	The simultaneous recognition mechanism of cations and anions using macrocyclic-iodine structures: insights from dispersion-corrected DFT calculations. *Physical Chemistry Chemical Physics*, **2020**, 22, 23795-23803	3.6	9
29	What is the driving force behind molecular triangles and their guests? A quantum chemical perspective about host-guest interactions. *Physical Chemistry Chemical Physics*, **2020**, 22, 19213-19222	3.6	2
28	An investigation of the photovoltaic parameters of ZnS grown on ZnO(101). *New Journal of Chemistry*, **2020**, 44, 20600-20609	3.6	0
27	On the recognition of chloride, bromide and nitrate anions by anthracene–squaramide conjugated compounds: a computational perspective. *New Journal of Chemistry*, **2020**, 44, 17831-17839	3.6	3
26	CO, NO, and SO adsorption on Ni nanoclusters: a DFT investigation. *Dalton Transactions*, **2020**, 49, 6407-6417	4.3	12

25	Double-bond elucidation for arsagermene with a tricoordinate germanium center: a theoretical survey. *New Journal of Chemistry*, **2019**, 43, 15681-15690	3.6	0
24	Adsorption of CO, NO, and H2 on the PdnAu55−n Nanoclusters: A Density Functional Theory Investigation within the van der Waals D3 Corrections. *Journal of Physical Chemistry C*, **2019**, 123, 7431-7439	3.8	11
23	Band alignment and charge transfer predictions of ZnO/ZnX (X = S, Se or Te) interfaces applied to solar cells: a PBE+U theoretical study. *Physical Chemistry Chemical Physics*, **2018**, 20, 4953-4961	3.6	13
22	Ab Initio Investigation of the Role of Atomic Radius in the Structural Formation of PtnTM55−n (TM = Y, Zr, Nb, Mo, and Tc) Nanoclusters. *Journal of Physical Chemistry C*, **2018**, 122, 7444-7454	3.8	12
21	Bare versus protected tetrairidium clusters by density functional theory. *Physical Chemistry Chemical Physics*, **2018**, 20, 29480-29492	3.6	2
20	Density functional investigation of the adsorption effects of PH and SH on the structure stability of the Au and Pt nanoclusters. *Journal of Chemical Physics*, **2017**, 146, 164304	3.9	7
19	Evolution of the structural, energetic, and electronic properties of the 3d, 4d, and 5d transition-metal clusters (30 TM systems for n = 2-15): a density functional theory investigation. *Physical Chemistry Chemical Physics*, **2017**, 19, 15484-15502	3.6	74
18	Theoretical Study of the Structural, Energetic, and Electronic Properties of 55-Atom Metal Nanoclusters: A DFT Investigation within van der Waals Corrections, Spin−Orbit Coupling, and PBE+U of 42 Metal Systems. *Journal of Physical Chemistry C*, **2016**, 120, 28844-28856	3.8	59
17	A theoretical investigation of the structural and electronic properties of 55-atom nanoclusters: The examples of Y-Tc and Pt. *Journal of Chemical Physics*, **2016**, 144, 054310	3.9	9
16	Structure, Electronic, and Magnetic Properties of Binary PtnTM55−n (TM = Fe, Co, Ni, Cu, Zn) Nanoclusters: A Density Functional Theory Investigation. *Journal of Physical Chemistry C*, **2015**, 119, 15669-15679	3.8	51
15	Atomic structure of the La/Pt(111) and Ce/Pt(111) surfaces revealed by DFT+U calculations. *RSC Advances*, **2015**, 5, 521-528	3.7	7
14	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, 11565-73	2.8	24
13	Structural formation of binary PtCu clusters: A density functional theory investigation. *Computational Materials Science*, **2015**, 98, 278-286	3.2	34
12	The role of charge states in the atomic structure of Cu(n) and Pt(n) (n = 2-14 atoms) clusters: a DFT investigation. *Journal of Physical Chemistry A*, **2014**, 118, 10813-21	2.8	77
11	Theoretical Investigation of Small Transition-Metal Clusters Supported on the CeO2(111) Surface. *Journal of Physical Chemistry C*, **2014**, 118, 21438-21446	3.8	29
10	Role of van der Waals corrections for the PtX2 (X=O, S, Se) compounds. *Physical Review B*, **2013**, 88,	3.3	23
9	Structural and electronic properties of TM23 - pAgp (TM = Ni, Pd, and Pt) clusters in the dilute limit (p = 0−4): A density functional theory investigation. *European Physical Journal D*, **2013**, 67, 1	1.3	13
8	Hybrid density functional study of small Rhn (n=2−15) clusters. *Physical Review B*, **2012**, 86,	3.3	32

7	Adsorption of NO on the Rh13, Pd13, Ir13, and Pt13 Clusters: A Density Functional Theory Investigation. *Journal of Physical Chemistry C*, **2012**, 116, 20540-20549	3.8	29
6	Platinum-Based Nanoalloys PtnTM55− (TM = Co, Rh, Au): A Density Functional Theory Investigation. *Journal of Physical Chemistry C*, **2012**, 116, 18432-18439	3.8	53
5	Bulk structures of PtO and PtO2 from density functional calculations. *Physical Review B*, **2011**, 84,	3.3	29
4	Transition-metal 13-atom clusters assessed with solid and surface-biased functionals. *Journal of Chemical Physics*, **2011**, 134, 134105	3.9	24
3	The role of electron localization in the atomic structure of transition-metal 13-atom clusters: the example of Co13, Rh13, and Hf13. *Physical Chemistry Chemical Physics*, **2011**, 13, 17242-8	3.6	38
2	Density functional theory investigation of 3d, 4d, and 5d 13-atom metal clusters. *Physical Review B*, **2010**, 81,	3.3	180
1	Reconstruction of core and surface nanoparticles: The example of Pt55 and Au55. *Physical Review B* , **2010**, 82,	3.3	50