# Maurcio Jeomar Piotrowski

## List of Publications by Citations



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|---|---|---|---|
| 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 | Density functional theory investigation of 3d, 4d, and 5d 13-atom metal clusters. *Physical Review B*, **2010**, 81, | 3.3 | 180 |
| 41 | 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 |
| 40 | 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 |
| 39 | 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 |
| 38 | 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 |
| 37 | Structure, Electronic, and Magnetic Properties of Binary PtnTM55□ (TM = Fe, Co, Ni, Cu, Zn) Nanoclusters: A Density Functional Theory Investigation. *Journal of Physical Chemistry C*, **2015**, 119, 15669-15679 | 3.8 | 51 |
| 36 | Reconstruction of core and surface nanoparticles: The example of Pt55 and Au55. *Physical Review B* , **2010**, 82, | 3.3 | 50 |
| 35 | 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 |
| 34 | Structural formation of binary PtCu clusters: A density functional theory investigation. *Computational Materials Science*, **2015**, 98, 278-286 | 3.2 | 34 |
| 33 | Hybrid density functional study of small Rhn (n=2□15) clusters. *Physical Review B*, **2012**, 86, | 3.3 | 32 |
| 32 | 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 |
| 31 | 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 |
| 30 | Bulk structures of PtO and PtO2 from density functional calculations. *Physical Review B*, **2011**, 84, | 3.3 | 29 |
| 29 | 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 |
| 28 | Transition-metal 13-atom clusters assessed with solid and surface-biased functionals. *Journal of Chemical Physics*, **2011**, 134, 134105 | 3.9 | 24 |
| 27 | Role of van der Waals corrections for the PtX2 (X=O, S, Se) compounds. *Physical Review B*, **2013**, 88, | 3.3 | 23 |
| 26 | 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 |

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| 25 | 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 |
| 24 | 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 |
| 23 | 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 |
| 22 | CO, NO, and SO adsorption on Ni nanoclusters: a DFT investigation. *Dalton Transactions*, **2020**, 49, 6407-6417 | 4.5 | 12 |
| 21 | 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 |
| 20 | Investigation of CO Adsorption on 13-Atom 4d Clusters. *Journal of Chemical Information and Modeling*, **2020**, 60, 537-545 | 6.1 | 11 |
| 19 | 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 |
| 18 | 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 |
| 17 | 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 |
| 16 | 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 |
| 15 | 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 |
| 14 | 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 |
| 13 | 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 |
| 12 | Tracking the role of trans-ligands in ruthenium–NO bond lability: computational insight. *New Journal of Chemistry*, **2020**, 44, 11448-11456 | 3.6 | 2 |
| 11 | 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 |
| 10 | 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 |
| 9 | Bare versus protected tetrairidium clusters by density functional theory. *Physical Chemistry Chemical Physics*, **2018**, 20, 29480-29492 | 3.6 | 2 |
| 8 | The anionic recognition mechanism based on polyol and boronic acid receptors. *New Journal of Chemistry*, **2020**, 44, 5564-5571 | 3.6 | 1 |

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| 7 | 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 |
| 6 | 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 |
| 5 | Double-bond elucidation for arsagermene with a tricoordinate germanium center: a theoretical survey. *New Journal of Chemistry*, **2019**, 43, 15681-15690 | 3.6 | 0 |
| 4 | Electrochemical, theoretical, and analytical investigation of the phenylurea herbicide fluometuron at a glassy carbon electrode. *Electrochimica Acta*, **2022**, 408, 139945 | 6.7 | 0 |
| 3 | 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 | 0 |
| 2 | An investigation of the photovoltaic parameters of ZnS grown on ZnO(101). *New Journal of Chemistry*, **2020**, 44, 20600-20609 | 3.6 | 0 |
| 1 | Designing boron and metal complexes for fluoride recognition: a computational perspective. *Physical Chemistry Chemical Physics*, **2021**, 23, 22768-22778 | 3.6 | |