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Binary Platinum-Based Nanoclusters: A Density Functional Theory Investigation[1] JUAREZ L.F. DA SILVA, São Carlos Institute of Chemistry, University of São Paulo, RICARDO K. NOMIYAMA, São Carlos School of Engineering, MAURÍCIO J. PIOTROWSKI, Federal University of Pelotas, DIEGO GUEDES SOBRINHO, São Carlos Institute of Chemistry, University of São Paulo, ANDERSON S. CHAVES, São Carlos Institute of Physics, University of São Paulo — Binary Ptatinum-based nanoclusters have attracted great attention in the last years due to the possibility to improve the chemical and physical properties of Pt nanoclusters. In this work, we will report a theoretical study of the structure and electronic properties of the Pt_nTM_{55-n} (TM = Fe, Co, Ni, Cu, Zn, Rh, Au) nanoclusters using density functional theory as implemented in the Vienna Ab-Initio Simulation Package (VASP). We found negative values for the excess energy for all systems, except for TM = Au, which indicates a gain in stability of the nanoclusters in comparison to the parent systems, i.e., Pt_{55} and TM_{55}. We observed that platinum has a strong preference to occupy the nanocluster surface, except for TM = Au, which can be explained by the large atomic radius of Pt atoms compared with with the Fe, Co, Ni, Cu, and Zn atoms. Our results indicate that the core-shell configuration, in which the core (13 TM atoms) and shell (42 Pt atoms) are from different chemical species, has greater stability compared with other compositions for all systems (except for TM = Au). Furthermore, we studied the average effective coordination, bond lengths, magnetic, and electronic properties of all those systems as a function of the composition.

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