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Electronic and structural properties of binary Pt-Ni nanoclusters
LUIS A. PÉREZ, IGNACIO L. GARZÓN, Instituto de Física, Universidad Nacional Autónoma de México — The lowest energy structures of binary $(PtNi_3)_n$, $(Pt_3Ni)_n$, and $(PtNi)_m$ nanoclusters, with n=3-10 and m=3-20, modeled by the many-body Gupta potential, were obtained by using a genetic-symbiotic algorithm. These structures were further relaxed with DFT-GGA. In agreement with the experimental evidence, segregation is observed in these clusters, where the Ni atoms are mainly found in the cluster core and the Pt atoms on the cluster surface. Furthermore, it has been experimentally found that the $(Pt_3Ni)_n$ nanoalloys present a higher catalytic activity for the $N_2O + H_2$ reaction at low temperatures than the other compositions [1], while the contrary trend is observed in the case of the oxidation of carbon monoxide in the presence of hydrogen, where the $(PtNi_3)_n$ nanoparticles present a higher catalytic activity than the other ones. In order to understand these tendencies in the catalytic activity, we performed an analysis of the surface electronic structure of the bimetallic Pt-Ni nanoclusters with the mentioned compositions, by means of first-principles density functional calculations. Acknowledgments: This work was supported by CONACyT No. 43414-F. [1] Arenas-Alatorre J, Avalos-Borja M, Diaz G J. Phys. Chem. B **109**, 2371 (2005).

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