

Abstract Submitted
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Density functional study of structural properties of bimetallic Pt-Ni nanoparticles¹ LUIS A. PEREZ, Instituto de Fisica, Universidad Nacional Autonoma de Mexico, KARO MICHAELIAN, IGNACIO L. GARZON, Instituto de Fisica, UNAM — A study has been made of the structures and energy ordering of the lowest-lying isomers of the bimetallic nanoparticles $(\text{PtNi}_3)_n$, $(\text{Pt}_3\text{Ni})_n$, and $(\text{PtNi})_n$, with $n=1-20$. The lowest energy structures of binary Pt-Ni nanoclusters, modeled by the many-body Gupta potential, were obtained by using a genetic-symbiotic algorithm. These structures were further reoptimized within the DFT-GGA framework. The Gupta potential parameters used for the Pt-Ni interaction are the geometric average of the Pt-Pt and Ni-Ni ones. In agreement with the experimental evidence, segregation is observed in the Pt-Ni clusters, with the Ni atoms in the core and the Pt atoms on the cluster surface, even for the $(\text{PtNi}_3)_n$ case. A discussion of segregation versus mixing effects will be presented.

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