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Compositional-Dependent Structural Analysis of Cu_xPt_{38-x} Nanoparticles JOSAFAT GUERRERO-JORDAN, Posgrado en Ciencias (Fisica), Universidad de Sonora, ROY L. JOHNSTON, School of Chemistry, University of Birmingham, ALVARO POSADA-AMARILLAS, Dept. Inv. en Fisica, Universidad de Sonora — We present an exhaustive study of the lowest energy Cu_xPt_{38-x} clusters structures obtained through a genetic algorithm, which incorporates the Gupta potential to mimic interatomic bonding. A symmetric parameterization of the Gupta potential was used including a weighting factor (w) in order to search for different potential energy surfaces describing 38-atom Cu-Pt nanoparticles. This weighting factor was varied from 0 to 1 in steps of 0.1 to obtain a structure map which provides information on the structural distribution in terms of the composition. According to this structure map, the most abundant structural motif corresponds to the truncated octahedron. Atomic segregation was maximum for w = 1.0. We also present the plot of excess energy as a function of the weighting factor values for the complete compositional range. The most stable structures were found for w = 0.0. The most relevant structures were chosen to be reoptimized by using the DFT method. We found that the interatomic distances changed compared to those obtained with the genetic algorithm.

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