

Theoretical investigation of free-standing CoPd nanoclusters as a function of cluster size and stoichiometry in the Pd-rich phase: Geometry, chemical order, magnetism, and metallic behavior

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We report on a study of the geometrical structure, magnetic properties, and metallic behavior of free-standing CoPd nanoclusters with $N=7, 13, 19, 23,$ and 26 atoms, as a function of cluster size and stoichiometry, in the Pd-rich phase. The investigated structures were obtained using a Gupta potential in combination with a genetic algorithm energy minimization. The electronic properties of the ground state geometrical structures were determined by solving a self-consistent spd tight-binding Hamiltonian. The metallic behavior was studied using Kubo's criterion. We tested our approach against benchmark SIESTA calculations for some of the small clusters investigated in the present work. We discuss the competition between segregation and mixing effects by means of an order parameter. The magnetic moments are analyzed in the context of the local chemical and atomic environments and we propose a simple empirical expression for the average magnetic moment per atom of these binary clusters. © 2