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Magnetic properties of ternary and quaternary transition metal nanoclusters JAIME SOUTO CASARES, JAMES CHELIKOWSKY, University of Austin at Texas — The magnetic properties of transition-metal nanostructures is a topic that has attracted much interest, mainly because of the dramatic difference that exists in comparison with the bulk. Without a proper knowledge of the fundamental mechanism behind the magnetic phenomena, it is hard to predict the properties of complex materials. We investigate the electronic and magnetic properties of nanoclusters made of ternary and quaternary compounds of transition metals (Fe, Co, and Ni) using PARSEC, a real-space implementation of pseudopotentials within density functional theory. Our code is well suited for the study of isolated structures because of its implementation of very efficient techniques for solving the Kohn-Sham equations. The real-space nature of PARSEC allows the use of proper boundary conditions, imposing the electronic wave functions to vanish outside a spherical domain. With these computational tools we can cover a wide spectrum of magnetic alloys and look for specific magnetic properties. This work is supported by NSF grant DMR 14-35219.

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