Magnetic properties of low-dimensional systems: confined atoms, small clusters, and nanoparticles with complex morphologies

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We present extensive calculations, using various theoretical models with different degrees of approximation, dedicated to analyze the electronic and magnetic properties of several low-dimensional systems. Following recent experimental findings, we analyze the stability and magnetic properties of polycrystalline cobalt nanoparticles and nanowires. We underline the importance of the local atomic environment in defining the low-energy orientation of the magnetization in the structures. Furthermore, by simulating the transmission microscopy images of these particles with complex morphologies, we provide well defined finger prints to identify precise details of the local atomic structure. We consider also Fe-Ni and Fe-Pd nanoparticle alloys. Based on a direct comparison with experiments, we determine the possible chemical order within the structures and evidence the crucial role played by the orbital-to-spin ratio in determining the location of the iron impurities within the particles. We discuss also the catalytic activity of both free-standing and carbon-supported small transition metal clusters. We consider the stability of Rh and Pt aggregates as well as their interaction with nitric oxide and hydrogen molecules. We analyze the conditions that need to be present to achieve the dissociation of the N-O and H-H bonds. Finally, we present our data for the encapsulation of magnetic atoms on spheroidal carbon cages. We discuss the possibility of controlling the local spin moment of the confined species by controlling its location within the cavity.