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Evolution of Magnetism from Atoms to Crystals[1]

MURILO TIAGO, University of Texas at Austin

The existence of spontaneous magnetization in metallic systems is an intriguing problem because of the extensive technological applications of magnetic phenomena and an incomplete theory of its fundamental mechanisms. Clusters of metallic atoms are important in this respect as they serve as a bridge between the atomic limit and the bulk, and they can form a basis for understanding the emergence of magnetization as a function of size. In solids, ferromagnetism is understood in terms of the exchange interaction and the formation of distinct energy bands for the majority spin and minority spin channels. In clusters, energy bands are replaced with dellocalized electronic orbitals, whose properties are affected by the finite size and the presence of a surface. Therefore, the size and shape of a cluster play important role in its magnetic properties. Indeed, direct measurements have indicated a strong dependence of magnetic moment with the size of the cluster, especially in iron clusters but also nickel and cobalt. Taking advantage of recent developments in computational methods for the electronic structure of nanosystems, we can now investigate in greater detail the magnetic properties of metallic clusters containing several hundreds of atoms and understand the role of size and shape. This analysis is based on first-principles density-functional theory, within the generalized gradient approximation. Numerical calculations were done in clusters containing up to 400 atoms (iron, nickel, and cobalt). Calculations are done using the PARSEC code (www.ices.utexas.edu/parsec). We also discuss some of the recently developed capabilities of PARSEC.

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