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Magnetic materials have received widespread interest due to their potential in technological applications ranging from biomedicine to data storage.[1, 2] Nanomaterials provide attractive platforms to build magnetic systems because they have been shown to exhibit enhanced per-atom magnetic moments relative to bulk.[3] Here, magnetic properties of Co_{13} and Co_{55} nanoclusters, passivated by surface ligand shells that exhibit varying electronic interactions with the metal, are studied using density functional theory. The calculations show that the chemical nature of the bond between the ligand and metal core (X-type or L-type) impacts that total magnetic moment of Co nanoclusters dramatically. Furthermore, the chemical identity of the ligand within each binding motif then provides a fine handle on the exhibited magnetic moment of the cluster. Thus, ligand shell chemistry is predicted to not only stabilize Co nanoclusters, but provide a powerful approach to control their magnetic properties, which combined enable a variety of magnetism-based applications.

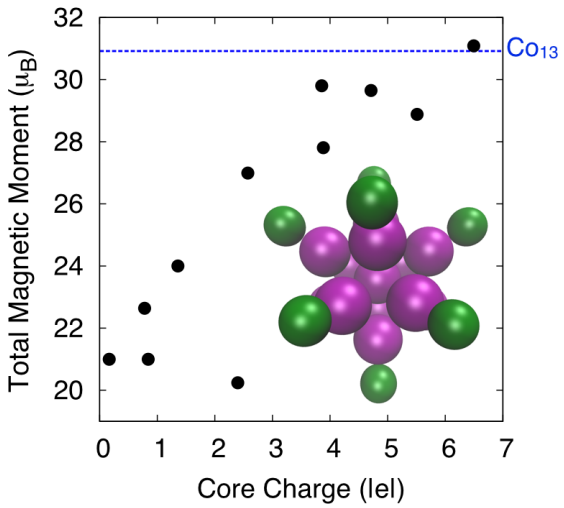

Figure 1: For $Co_{13}X_{12}$ nanoclusters, the charge on the Co13 core controls the total magnetic moment of the cluster.

References:

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