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Correlation effects on the properties of small cobalt clusters
YVETTE HANCOCK, MARI IJÄS, Department of Engineering Physics, Helsinki University of Technology, Finland — Demands for higher-density magnetic storage media and smaller memory devices require atomic-scale magnetic components with stable magnetic properties. One such candidate for this application is a small transition metal cluster. The magnetic properties of transition metal clusters are very sensitive to the geometry of the cluster, the local atomic and structural environments, and to the system size. In this work, the GGA + U DFT approach is used for the first time to study the system properties of small cobalt clusters consisting of 2 to 5 atoms. Previous studies using DFT and tight-binding approaches have been found to overestimate the binding energies, dissociation energies and vibrational frequencies of the clusters against their known experimental values. By including a Hubbard U correction between 2 – 3 eV, the DFT method can then be fitted to reproduce the experimental results, thereby improving upon previous theoretical descriptions of these systems. The effect of U on the calculated magnetic and structural properties of the clusters is also discussed.

Yvette Hancock
Department of Engineering Physics, Helsinki University of Technology

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