Density functional calculations of Au_3Co

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The investigation of magnetic properties and the electronic structure of cobalt atom in different chemical and structural environment is a fascinating field of research. In the present work, we modelled the hypothetical Au_3Co theoretical compound, where the Co atom is surrounded by three gold atoms as a model for high Co concentration in gold. The magnetic properties of the Co atom in this structure have been calculated in the framework of local spin density approximation (LSDA) using the relativistic version of the full-potential local orbital minimum basis code. We also compare the two different approaches to calculate the magnetocrystalline anisotropy energy called the total energy approach and the force theorem approach.

9.7 cm

13.4 cm

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