Magnetism from first-principles

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ABSTRACT

Development and engineering of new magnetic materials is one of the main goals in modern condensed matter physics. Thereby, first-principles simulations play a significant role in the design of new materials. Nowadays first-principles methods based on the density functional theory can provide very accurate information about electronic and magnetic properties of realistic systems and has become a major supplement and alternative to the experiment.
In my talk I present a first-principles approach, based on the multiple-scattering theory, which provides explicitly the Green function that can be used in many applications such as spectroscopy, transport, and many-body physics. Combined with the coherent-potential approximation this method can be used as well for the description of alloys and pseudo-alloys. In my presentation, I shall focus on applications of our approach in magnetism, in particular, of low dimensional systems such as single magnetic atoms on metallic surfaces, magnetic thin films, and disordered materials.