Effective magnetic Hamiltonians

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Abstract

Based on the first-principles electronic-structure calculations, we construct the effective magnetic Hamiltonians that can be used to search for the ground state of solids and nanostructures. Using the methods of statistical mechanics, one can study the magnetic properties such as the magnetic structure as a function of temperature, magnon spectra, the Curie/Néel temperature, etc. The present approach is highly flexible and it makes possible to study magnetic structure of complex systems with the accuracy of ab initio methods. Simultaneous treatment of local exchange interactions and the interatomic exchange interactions makes possible to correctly describe the varying values of magnetic moments and origin of induced magnetic moments. We will show the construction of the effective magnetic Hamiltonian for 3d and 4d metals and their alloys, and the importance of anisotropic interactions for determination of the magnetic structure of magnetic monolayers on non-magnetic substrates, e.g., a magnetic monolayer (Fe) on a non-magnetic substrate (Ir(001)).