

Constituents of magnetic anisotropy and screening of spin orbital coupling in magnets

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We propose a new quantum mechanical scheme to analyze the origin and spatial distribution of magnetic anisotropy in itinerant and correlated magnets. This method uses approximate perturbation theory and exact integration over parameter techniques. A simple relation between a total magnetic anisotropy and spin orbital coupling anisotropy has been obtained for different crystal symmetries. We analyze the effective screening of spin orbital coupling in solids and demonstrate practical use of this effect. A novel version of the virial theorem has been introduced to analyze separate contributions to magnetic anisotropy from kinetic, potential and spin orbital coupling terms in the effective Hamiltonian. This theory has been applied for many popular magnets: FePt, CoPt, MnBi, MnAl, FeNi, where a microscopic explanation of high anisotropy has been obtained. This analysis has shown that in the itinerant magnets there is very strong intersite orbital anisotropic interactions, that often provide unexpected large and dominant contributions to magnetic anisotropy. We have shown that single-ion anisotropy model is not suitable for many itinerant magnets, while an addition of two-ion anisotropy, due to large orbital interatomic coupling, creates a very consistent description of anisotropic magnetic properties. An extension of proposed technique for the implementation in the many body methods is proposed.

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