Crystal field and magnetism with Wannier functions: rare-earth intermetallics and low symmetry systems

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Until recently no robust ab-initio method to calculate the crystal field of rare-earth ions in crystals was available. During the last two years we developed a scheme, which was succesfuly used to determine the crystal field parameters of trivalent RE ions in oxides with orthoperovskite and garnet crystal structure. These parameters were then inserted in atomic-like program which, besides the crystal field, takes into account the 4f-4f electron repulsion, spin-orbit and Zeeman interactions. The agreement of the calculated and experimental splitting of RE multiplets was very good (within meV) and also magnetism of the RE multiplet is correctly described.

The method uses the density functional theory based band structure calculation, followed by a transformation of the Bloch to the Wannier basis and expansion of the local Hamiltonian in terms of the spherical tensor operators. It contains a single adjustable parameter that characterizes the hybridization of RE(4f) states with the states of oxygen ligands. In the present contribution the method is applied to $NdFe_{14}B$ and to R:LaF_3 (R=Ce, Pr, ... Yb). In LaF_3 the rare earth site has a low symmetry and 27 crystal field parameters are needed to describe the crystal field.