Crystal field and magnetism with Wannier functions

A talk by Pavel Novak
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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 more than fifty oxides and in lanthanum trifluoride. These parameters are then inserted in an 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 is 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 form the method may be applied to an arbitrary local symmetry of the RE site and the demands on computer power are moderate. We believe that it may become an important tool for understanding and predicting the physics of rare-earth compounds.