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# Crystal field and magnetism with Wannier functions: rare-earth ions in garnets, manganites and cobaltates

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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 orthoaluminates and cobaltites with orthorhombic perovskite 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 ground RE multiplet was correctly described.

In the present contribution the application of the method to rare-earth manganites is briefly described, including comparison of calculated and experimental g-factors of the RE excited states. The results obtained for Pr and Nd layered cobaltates are also presented. Our main focus is, however, on the yttrium aluminium and lutetium aluminium garnets, which contain RE as an impurity. For these systems plentiful and reliable experimental optical absorption spectra and EPR data exist. Comparison with the calculated results allows to assess accuracy and limits of the method and indicates that it can well be used to predict energy levels and magnetism of the rare-earth ions in crystals.

P. Novák, K. Knížek and J. Kuneš, Phys. Rev. B **87**, 205139 (2013).
P. Novák, K. Knížek, M. Maryško, Z. Jirák and J. Kuneš, J. Phys.: Condens. Matter **25**, 446001 (2013).