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Calculation of crystal field parameters with Wannier functions

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Calculation of the crystal field parameters (CFP) of the rare-earth (RE) ions in solids is a formidable problem and until recently no robust ab-initio method to calculate them was available. The main problem is that in most approaches the 4f electrons of RE are allowed to interact with the nonspherical electron density they create themselves and this false selfinteraction completely distorts the crystal field. The second problem is that no ab-initio method is capable to determine correctly hybridization of the 4f levels with ligand electron states. In this contribution we describe how the problem of the selfinteraction may be avoided, while the problem of the hybridization is circumvented by introducing single parameter, value of which may be estimated from the experiment. To calculate the electron structure the WIEN2k package is employed. After removing the selfinteraction, CFP are determined from 4f Wannier functions. Method is applied to $TbAlO_3$, for which set of CFP was determined recently and to $YAlO_3$ with small substitution of Y by RE (RE= Ce, ..., Yb). These systems are frequently studied laser materials and a number of relevant experimental data exist. In $REMO_3$ compounds (M=Ga, Co) the magnetic susceptibility is calculated and compared with the experimental results. The agreement between theory and experiment is in all cases very good, indicating that crystal field parameters in oxides can be calculated with an accuracy which allows reliable prediction of the rare-earth energy levels and magnetism.

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[2] P. Novák, K. Knížek and J. Kuneš, Phys. Rev. B **87**, 205139 (2013).
[3] P. Novák, K. Knížek, M. Maryško, Z. Jirák and J. Kuneš, J. Phys.: Condens. Matter (in print).