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Calculation of crystal field parameters

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Abstract. Calculation of the crystal field parameters (CFP) of the rare earth (RE) ions in solids is a formidable problem and until now no robust ab-initio method to calculate them is 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 the position of the 4f levels relative to other electron states. In this contribution we describe how the problem of the selfinteraction may be avoided, while the problem of the 4f position is circumvented by introducing single parameter, value of which is estimated using a semiempirical approach. The method is first tested on Pr^{4+} ion in cubic praseodymium dioxide and then 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. To calculate the electron structure the WIEN2k package is employed. After removing the selfinteraction, CFP are determined from the RE 4f Wannier functions. The method is compared to other approaches of CFP calculation and its limitations are discussed.