View Abstract

CONTROL ID: 3464947

TITLE: DFT-based Calculations of the Magnetic Hyperfine Interactions at Cd Sites in RECd Compounds with the FP-LAPW ELK Code

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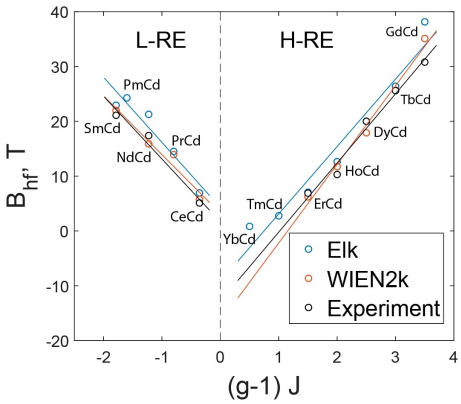

Fig. 1: Spin dependence of hyperfine magnetic field at Cd sites obtained with the ELK and WIEN2k codes and in the TDPAC experiment, and their linear fits.

ABSTRACT BODY:

Abstract Body: In this work we tested the methodology to map magnetic hyperfine interactions in strongly correlated materials using a free open-source all-electron FP-LAPW code ELK. The RECd (RE = Ce, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb) series was chosen as a laboratory system, since an almost complete set of experimental data on the hyperfine parameters at Cd sites in these compounds was acquired previously with an extremely sensitive TDPAC technique [1]. Moreover, these TDPAC results were complemented with WIEN2k DFT calculations that allow a qualitative comparison of the two codes. The ELK calculations were performed with PBE96 GGA-type exchange-correlation functional, the cases of scalar relativistic approximation and fully relativistic relaxation of the states were treated separately. A dense *k*-mesh and adequate $R_{MT}K_{max}$ were chosen in both cases to comply with the sensitivity of magnetic hyperfine parameters.
We emphasize that the exploited version of ELK accounted for the contact field only. Yet, as it is the only contribution expected for Cd site in RECd, the values of B_{hf}, albeit generally overestimated, have shown reasonable agreement with the experiment (Fig. 1). Spin-orbit coupling taken into account led to a decrease in deviation from experimental data. An addition of the Hubbard-like term was essential to reach a tolerable result for CeCd. This behavior may be associated with a weaker localization of the 4f electron of Ce.
Concerning the potential sources of discrepancy between our ELK results and those previously obtained with WIEN2k, (i) a different way of accounting for relativistic corrections, (ii) the use of GGA (our ELK study) versus LDA (previous WIEN2k study) and other details are discussed.

References: [1] F. H. M. Cavalcante et al. Phys. Rev. B, Vol. 94, 064417 (2016)

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