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Magnetic anisotropy of rare-earth magnets calculated by SIC and OEP[1] HISAZUMI AKAI, ISSP, Univ of Tokyo, MASAKO OGURA, PGI, Juelich Research Center — We have pointed out in our previous study that the chemical bonding between N and Sm plays an important role in the magnetic anisotropy change of Sm_2Fe_{17} from in-plane to uniaxial ones caused by the introducing of N. This effect of N insertion was discussed in terms of change in the electronic structure calculated in the framework of LDA+SIC. The main issue here is whether the 4f states are dealt with properly in SIC. In the present study, we examine the applicability of SIC for the evaluation of the magnetic anisotropy of rare-earth (RE) magnets by comparing the results with various methods, in particular, the optimized effective potential (OEP) method. In this study, OEP is applied only on the RE sites. Admittedly, this is a drawback from the viewpoint of the consistent treatment of uncertainly inherent in the so-called KLI (Krieger-Li-Iafrate) constants. Putting this aside for the moment, we have calculated the electronic structure of RE magnets $R_2Fe_{17}N_x$ and RCo_5 (R=light RE), by OEP with exact-exchange (EXX) combined with Colle-Salvetti correlation. Our preliminary results have shown considerable differences between the SIC and OEP calculations. We will discuss the meaning of this discrepancy.

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