Abstract Submitted
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Constituents of magnetic anisotropy and a screening of spin-orbit coupling[1] LIQIN KE, ALEKSANDER WYSOCKI, Ames Laboratory USDOE, MARK VAN SCHILFGAARDE, Department of Physics, King's College London, VLADIMIR ANTROPOV, Ames Laboratory USDOE — Using perturbation theory (PT) we analyze how the different orders of perturbation affect the energy in solids. We test the validity of PT analysis by considering spin-orbit coupling (SOC) as a perturbation. We show how the atomic SOC is screened in different magnets and how it affects the magnetic anisotropy. The dependence of magnetic anisotropy on the ratio between the strengths of SOC and crystal field is studied using an impurity model. We carried out density functional calculations for FePt, CoPt, FePd, MnAl, MnGa, FeNi, and tetragonally strained FeCo. The relativistic energy and magnetic anisotropy in those compounds from the perturbation approach and self-consistent relativistic calculations had been compared. In addition using decomposition of anisotropy into contributions from individual sites and different spin components we explain the microscopic origin of high anisotropy in most popular magnets.

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