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Dissecting the mechanisms of magnetocrystalline anisotropy in alloys: Electronic structure analysis tools and applications to $(Fe_{1-x}Co_x)_2B$ and $Li_{3-x}Fe_xN$ alloys[1] KIRILL BELASHCHENKO, University of Nebraska - Lincoln, VLADIMIR ANTROPOV, Ames Laboratory — We describe a first-principles code and a set of tools providing detailed information about the mechanisms of the magnetocrystalline anisotropy (MCA) in alloys. The spin-orbit coupling (SOC) is included in the Green's function-based linear muffin-tin orbital (LMTO) method combined with the coherent potential approximation. Third-order correspondence with the LMTO Hamiltonian is formally demonstrated. The analysis tools include the identification of contributions from different spin channels, single-ion and two-ion terms and alloy components by computing the SOC energy with scaled SOC parameters, as well as a full reciprocal-space resolution of MCA in the Brillouin zone. Application of these tools is illustrated for the $(Fe_{1-x}Co_x)_2B$ system, where the complicated non-monotonic concentration dependence of MCA is attributed to the combination of band filling and SOC selection rules. For $Li_{3-x}Fe_xN$ we demonstrate the interplay between chemical disorder, orbital polarization, and correlation effects in a doubly degenerate impurity band.

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