# Magnetic properties of FeB and MnB doped with 3$d$, 4$d$ and 5$d$ transition metal elements

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The increasing use of magnetically hard materials in industry, together with the unstable prices of rare earths observed over the past several years, is mobilizing the search for new materials that could, albeit in specific applications, replace rare earth-containing magnets. Of the Mn- and Fe-rich compounds under consideration, the notable ones, in our opinion, are MnB and FeB monoborides and their alloys. In this paper, using first-principles calculation methods, we systematically study MnB and FeB alloys with 3$d$, 4$d$ and 5$d$ transition metals (TM) [1-2]. We consider compositions with the general chemical formula of $Mn_{11}(TM)_1B_{12}$ and $Fe_{11}(TM)_1B_{12}$. In our calculation magnetocrystalline anisotropy energy (MAE), magnetic moments, and magnetic hardness are determined for all compositions considered. Moreover, the calculated dependence of MAE on the spin magnetic moment made it possible to predict the upper limits of the MAE. We have also shown within the virtual crystal approximation that the magnetic moments on magnetic atoms strongly depend on the electron occupancy, which is modified by both the substitution and the strong interaction between the (Mn/Fe) − 3$d$ and B − 2$p$ orbitals. This interaction leads to a shift in the Bethe-Slater curve, showing the dependence of transition metal exchange energy on $d$-band occupation. This mixing of p − d orbitals, resulting from the redistribution of band occupancy, also leads to strain-induced MAE changes. We have also selected few materials with potential of becoming rare-earth free permanent magnets such as $Fe_{11}TiB_{12}$ for which we have obtained value of MAE equal 0.86 $\mathrm{MJ\,m^{-3}}$ and magnetic hardness equal 1.15.

Calculations were performed using the full-potential local-orbital electronic structure code FPLO18 [3], whose unique fully relativistic implementation of the fixed spin moment method allowed the calculation of the MAE dependence of the magnetic moment.

**References:**

[1] J. Snarski-Adamski and M. Werwiński, *J. Magn. Magn. Mater.*, 169309 (2022)
[2] J. Snarski-Adamski, J. Rychły, and M. Werwiński, *J. Magn. Magn. Mater.*, 168828 (2022)
[3] K. Koepernik, H. Eschrig, *Phys. Rev. B.* 59, 1743 (1999)

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