Ab initio studies of selected Fe/Co alloys for permanent magnet applications

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The $(Fe_{1-x}Co_x)_2B$ [1], $(Fe_{1-x}Co_x)_5SiB_2$ [2], and $(Fe_{1-x}Co_x)_5PB_2$ alloys have been investigated theoretically as candidates for rare-earth free permanent magnets. Magnetocrystalline anisotropy energies MAE, identified as the leading magnetocrystalline anisotropy constants K_u, have been calculated with the virtual crystal and coherent potential approximations (VCA and CPA) for a full range of Fe/Co compositions. The variations of MAE versus magnetization have been addressed with a full relativistic fixed spin moment method. The optimal compositions with the highest MAE's were determined. The *ab initio* results have been confronted with experiment.

References:

[1] A. Edström et al. Phys. Rev. B 92, 174413 (2015)

[2] M. Werwiński et al., Phys. Rev. B 93, 174412 (2016)

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