Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

First-principles study of intrinsic magnetic properties of hexagonal and orthorhombic $(Fe_{1-x}Co_x)_2P$ alloys[1] IVAN ZHURAVLEV, University of Nebraska-Lincoln, V. P. ANTROPOV, Ames Laboratory, K. D. BELASHCHENKO, University of Nebraska-Lincoln — $(Fe_{1-x}Co_x)_2P$ is a candidate rare-earth-free alloy for permanent-magnet applications, which is hexagonal (h) up to $x \approx 0.12$ and orthorhombic (o) at larger x. The Curie temperature T_C, which is only 270 K in Fe_2P, raises sharply with x, peaking above 450 K in the o-phase [1]. The measurement [2] of magnetocrystalline anisotropy (MCA) in the o-phase is inconsistent with Mössbauer data suggesting a spin reorientation transition (SRT) at $x \approx 0.3$ [1]. Here we report the results of *ab initio* calculations of the magnetization, mean-field T_C, and MCA in h- and o-phases as a function of x, addressing the role of unequal site occupation, which is confirmed by total-energy calculations. The trends in the magnetization are reproduced, as well as MCA in the h-phase, and so is the SRT near $x \approx 0.3$ (at odds with the results of Ref. 2). The trends in the mean-field T_C, obtained using the disordered-local-moment method, agree with experimental data. [1] R. Fruchart *et al.*, J. Appl. Phys. 40, 1250 (1969). [2] T. Hokabe *et al.*, J. Phys. Soc. Japan 36, 1704 (1974).

[1]Work at UNL is supported by NSF Grant DMR-1308751.

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Date submitted: 06 Nov 2015 Electronic form version 1.4