Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Large magnetic anisotropy predicted for metastable structures of rare-earth free Co-Fe-N compounds XIN ZHAO, CAI-ZHUANG WANG, LIQIN KE, YONGXIN YAO, KAI-MING HO, Ames Lab and Iowa State University
— Metastable structures of cobalt nitrides and Fe-substituted cobalt nitrides are explored as promising candidates for rare-earth free permanent magnets. Through crystal structure searches using adaptive genetic algorithm, new structures of Co_nN ($n = 3...8$) are found to have lower energies than those previously discovered by experiments. Substituting a fraction of Co with Fe helps to stabilize the new structures and at the same time further improve the magnetic properties. Based on first-principles density functional calculation, large magnetic anisotropy energy is predicted in this system, reaching as high as 3.18 MJ/m^3 (245.6 μeV per transition metal atom). In addition, for the extensively studied $Fe_{16}N_2$ magnets, we discuss a tetragonal to cubic structure transition as replacing Fe with Co, which can be well explained by electron counting analysis. Different magnetic properties in $Co_{16-x}Fe_xN_2$ between the Co-rich side ($x \leq 8$) and Fe-rich side ($x > 8$) is closely related to the structural transition.

Xin Zhao
Ames Lab and Iowa State University

Date submitted: 12 Nov 2016 Electronic form version 1.4