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Origin and tuning of the magnetic anisotropy in Fe_2P-based alloys[1] IVAN ZHURAVLEV, Department of Physics and Astronomy, University of Nebraska-Lincoln, V.P. ANTROPOV, Ames Laboratory, U.S. Department of Energy, Ames, Iowa 50011, USA, K. D. BELASHCHENKO, Department of Physics and Astronomy, University of Nebraska-Lincoln — Fe_2P-based alloys have been studied for years due to their potential magnetocaloric applications. In addition, Fe_2P demonstrates record-high magnetocrystalline anisotropy (MCA) for systems with no heavy elements. While the Curie temperature T_C in pure Fe_2P is too low for applications, this system appears to be highly tunable, and its T_C can be greatly increased by alloying with many other d and p elements. Here we present the electronic structure analysis of magnetic properties of these alloys, searching for systems with higher T_C while preserving high MCA. The microscopic origin of the dominant contribution to MCA and its concentration dependence is revealed. We further find that co-alloying with Co or Ni and Si is a promising strategy for achieving high Curie temperature and MCA, which is more favorable compared to individual alloying by Co/Ni or Si due to the compensation of their effects on the band occupation.

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Ivan Zhuravlev
Department of Physics and Astronomy, University of Nebraska-Lincoln

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