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FeCo-based permanent magnet materials search by genetic algorithm CAI-ZHUANG WANG, MANH CUONG NGUYEN, XIN ZHAO, KAI-MING HO, Ames Laboratory, US DOE and Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA — FeCo alloy is well-known soft magnetic material with high magnetic moment, 2.5 μ_B/atom at $\sim$ 30 wt. % Co. However, doping FeCo alloys with heavy 5d transition metal and mix FeCo phase with nomagnetic structure of AlNi (e.g., Alnico) would increase the coercivity of the alloys. In order to gain more insight into the enhancement of the magnetic anisotropy in FeCo by doping or mixing, we have investigated the stable and metastable crystal structures of Fe-Co-W and Fe-Co-Al-Ni systematically over a wider range of composition by adaptive genetic algorithm method. Our search results show that the Fe-rich FeCoW alloys are all in bcc structures with W prefer substituting Fe sites. The Fe-Co-Al-Ni structures are also found to be in bcc lattice with broad chemical variation across the FeCo and AlNi interface. The magnetic properties in these stable and metastable structures are also calculated and the microscopic mechanism for the enhancement of magnetic anisotropy is discussed.

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