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Atomic Structures and Magnetic Properties of Fe-rich $Fe_{1-x}Co_x$ Alloys: A Genetic Algorithm Search MANH CUONG NGUYEN, XIN ZHAO, MIN JI, BRUCE HARMON, CAI-ZHUANG WANG, KAI-MING HO, Ames Laboratory, US DOE and Department of Physics and Astronomy, Iowa State University — Using genetic algorithm with first-principles calculations, we performed a broad global search for low-energy crystal structures of Fe-rich $Fe_{1-x}Co_x$ alloys. We found that Fe-rich $Fe_{1-x}Co_x$ alloys are highly configurationally degenerate and there are many additional off-stoichiometric stable structures to the well-known stoichiometric FeCo - B_2 structure, giving a possibility for atomistic manipulation of the alloys. The Co-Co nearest-neighbor pair is strongly unfavorable in Fe-rich $Fe_{1-x}Co_x$ alloys. The magnetic moment of Fe atom is increasing with Co concentration while that of Co atom is almost constant, inducing a Slater-Pauling curve for magnetic moment per atom. The magnetic moment of Fe atom is strongly dependent on the number of Co nearest-neighbors and it increases with this number.

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