

Abstract Submitted  
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**Magnetic properties of doped  $\text{Ce}_2\text{Co}_{17}$  alloys** LIQIN KE, DENIS KUKUSTA<sup>1</sup>, VLADIMIR ANTROPOV, Ames Laboratory USDOE, Ames, IA 50011 — Substitutional alloys  $\text{Ce}_2\text{Co}_{17-x}\text{T}_x$ , where T is *d*-atom or Al, Si, Ga, have been analyzed using electronic structure calculations with a focus on the influence of doping on such properties as magnetization, magnetic anisotropy and Curie temperature. A complication arises because we need to improve all three of these key properties of magnets. We found that a system with small levels of doping has a strong site preference effect. This effect, when combined with site decomposition of magnetic anisotropy and Curie temperature leads to the specific scenario of producing desirable new magnetic materials with better properties as permanent magnets. We show that in order to obtain a better set of these three key magnetic properties, one has to consider dopings by two elements, with one element responsible for changes to magnetic anisotropy and another for improving the magnetization and Curie temperature. Obtained theoretical results have been compared favorably with a large amount of available experimental data for certain systems.

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