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Rare-earth element based permanent magnets: a theoretical investigation[1] RAJIV K CHOUHAN, DURGA PAUDYAL, Ames Laboratory, U S department of Energy, Iowa State University, Ames, IA 50011 — Permanent magnetic materials with large magnetization and high magnetocrystalline anisotropy are important for technical applications. In this context rare-earth (R) element based materials are good candidates because of their localized $4f$ electrons. The $4f$ crystal field splitting provides large part of magnetic anisotropy depending upon the crystal environment. The d spin orbit coupling of alloyed transition metal component provides additional anisotropy. RCo_5 and its derivative R_2Co_{17} are known compounds for large magnetic anisotropy. Here we have performed electronic structure calculations to predict new materials in this class by employing site substitutions. In these investigations, we have performed density functional theory including on-site electron correlation (DFT+U) and L-S coupling calculations. The results show that the abundant Ce substitution in R sites and Ti/Zr substitutions in some of the Co sites help reduce criticality without substantially affecting the magnetic moment and magnetic anisotropy in these materials.

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