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Tailoring of $SmCo_5$ for optimal structure, magnetic anisotropy, and reduced criticality[1] DURGA PAUDYAL, R. CHOUHAN, The Ames Laboratory, Iowa State University, Ames, IA 50011, K. A. GSCHNEIDNER, JR., The Ames Laboratory and Department of Materials Science and Engineering, Iowa State University, Ames, IA 50011 — $SmCo_5$ forms hexagonal $CaCu_5$-type structure with three non-equivalent sites: Sm (1a), Co (2c), and Co (3g). Sm lies in the middle of the Co (2c) hexagonal layers. Advanced density functional theory calculations employing Hubbard model show crystal field split localized Sm 4f states, which are responsible for the large part of the magnetic anisotropy exhibited by this system. In addition, the hexagonal Co (2c) layers help enhancing the anisotropy. Due to the partially quenched Sm 4f orbital moment, there is a net Sm 4f moment, which also helps enhancing magnetic moment. The substitution of some of the Sm sites by Nd adds Nd 4f multiplet thereby enhancing crystal field split 4f states and overall magnetic moment. The substitution of Co (2c) by Fe is preferred over Co (3g) but the compound becomes chemically unstable. The criticality issues could be addressed by substituting abundant Ce.

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