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Site specific physics in RT_5 (R = rare earths and T = transition metals) materials[1] DURGA PAUDYAL, Ames Laboratory, Iowa State University, Ames, IA 50011 — Most of RT_5 compounds form in hexagonal $CaCu_5$-type structure with three non-equivalent sites: R (1a), T (2c), and T (3g). R atoms sit in the middle of the T (2c) hexagonal layers. Advanced density functional theory calculations including on-site electron correlation and spin orbit coupling show crystal field split localized R 4f states, which are responsible for the large part of the magnetic anisotropy exhibited by these systems. In addition, the hexagonal T (2c) layers help enhancing the magnetic anisotropy. Partially quenched R 4f orbital moment is the origin of magnetic anisotropy which also helps enhancing magnetic moment. The interchange of T sites by other transition metals and the partial substitution of R atoms by transition metals could optimize needed magnetic moment and magnetic anisotropy by forming a complex geometry structure favoring permanent magnetic properties.

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Durga Paudyal
Ames Laboratory, Iowa State University, Ames, IA 50011

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