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Magnetocrystalline anisotropy and magnetic properties of rare-earth dialuminides.[1] TIMOTHY HACKETT, D. PAUDYAL, V. K. PECHARSKY, Ames Laboratory, Ames, IA 50011, USA — We report here how the electronic structure and magnetocrystalline anisotropy play a role in the magnetic and structural transformations of rare-earth dialuminides. In addition, we also present the delicate balance between the spin and orbital magnetic moments and their effect on these transformations. We have employed predictive advanced density functional theory calculations including Hubbard model for onsite 4f electron correlation and spin orbit coupling for magnetocrystalline anisotropy. The predicted magnetostructural properties have been validated from experiments. Although the cubic Laves phase structure is fairly isotropic, our theoretical and experimental studies reveal that most of the rare earth dialuminides undergo high temperature paramagnetic to the low temperature ferromagnetic transition with coupled or decoupled structural transformations. Calculations show that crystal field split localized 4f and crystal field and exchange split delocalized 5d states are responsible for the magnetostructural transformations in these dialuminides.

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