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Unusual physical behaviors of strongly correlated rare earth dialuminides[1] DURGA PAUDYAL, The Ames Laboratory, U. S. Department of Energy, Iowa State University, Ames, IA 50011, V.K. PECHARSKY, K.A. GSCHNEIDNER, JR., The Ames Laboratory, U. S. Department of Energy and Department of Materials Science and Engineering, Iowa State University, Ames, IA 50011 — We present electronic, magnetic, and magnetostructural behaviors of rare earth dialuminides calculated by first principles. Total energy calculations show that $CeAl_2$ and $EuAl_2$ adopt antiferromagnetic ground states while dialuminides formed by other magnetic lanthanides have ferromagnetic ground states. The magnetic moment of $CeAl_2$ indicates that the 4f orbital moment of Ce in $CeAl_2$ is quenched. Eu in $EuAl_2$ and Yb in $YbAl_2$ are divalent. $PrAl_2$ exhibits a tetragonal distortion near ferromagnetic transition. $HoAl_2$ shows a first order magnetostructural transformation while $DyAl_2$ shows a second order transformation. The dialuminides formed by Nd, Tb, and Er are simple ferromagnet without additional anomalies in the ferromagnetic state. $SmAl_2$ orders ferromagnetically with less than 1 μ_B indicating the cancellation of 4f spin moment by its orbital counterpart. Due to substantially high 4f crystal field splitting $TmAl_2$ shows 4f spin magnetic moment lower than expected.

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