Abstract Submitted
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Interplay between magnetostructural transformation and magnetocrystalline anisotropy in $TbMn_2$[1] MANISH K. KASHYAP, D. PAUDYAL, B. N. HARMON, Ames Laboratory, U.S. Department of Energy, Iowa State University, Ames, Iowa 50011-3020 — Using density functional theory (DFT) approach, the magnetostructural phase transformations from paramagnetic cubic to ferrimagnetic rhombohedral structure in ordered and disordered $TbMn_2$ Laves phase compounds have been investigated. The calculations of the electronic and magnetic properties of these compounds were performed using the full potential linear augmented plane wave (FPLAPW) method. The added onsite electron correlation in local spin density approximation (LSDA+U) for the occupied and unoccupied $4f$-states yields a better representation of the bandstructure, density of states, and individual magnetic moments as compared to LSDA alone. Indirect $4f$-$4f$ exchange interactions and crystal field splitting play a significant role to decide magnetic and structural phases. Our results confirm the magnetocrystalline anisotropy driven rhombohedral ground state in $TbMn_2$.

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