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Understanding the interplay between crystal structures and magnetic states of RCo_2 (R = heavy rare earths)[1]
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The RCo_2 compounds with R = heavy lanthanides are well known model systems for both experimentalists and theorists because of the complex nature of the magnetism of these materials. Better understanding of the magnetism can be achieved from parameter-free first principles calculations as well as carefully executed experiments. From first principles calculations we show that the indirect $4f$- $4f$ exchange polarizes the $5d$ spins and the spin up $5d$ and spin down $3d$ hybridization gives rise to ferrimagnetism, i.e. antiparallel $5d$ and $3d$ itinerant magnetic moments at low temperature. The itinerant electron metamagnetism is known to support first order phase transformations in some of the RCo_2 compounds. However the clear understanding of this mechanism is lacking and, therefore, we clarify this mechanism from first principles calculations and experimentally confirm the nature of phase transformation of $TbCo_2$. The interrelation between the crystal structure and the magnetic states has also been investigated considering $TbCo_2$ as an example.

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