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Magnetic properties of $Ce(Fe_{1-x}Co_x)_{11}Ti$ and effects of H and N doping[1] LIQIN KE, VLADIMIR ANTROPOV, Ames Laboratory — The intrinsic magnetic properties of $Ce(Fe_{1-x}Co_x)_{11}Ti$ related systems have been studied using electronic structure calculations. Both $CeFe_{11}Ti$ and $CeCo_{11}Ti$ have uniaxial magnetic anisotropy. Calculations of the magnetic anisotropy of $Ce(Fe_{1-x}Co_x)_{11}Ti$ show that the easy magnetization direction changes from uniaxial to in-plane and then back to uniaxial with increasing Co content. This provides an explanation for the interesting non-monotonic behavior of coercivity observed in experiments. The effects of H and N doping on intrinsic magnetic properties are also studied. Both H and N doping increase the magnetization and Curie temperature while N doping has a stronger effect than H doping. Calculated T_C enhancements agree well with experiments and it is found that volume and chemical effects contribute nearly equally to the T_C enhancement with N doping. The uniaxial magnetic anisotropy decreases with N doping, which is consistent with experiments. However, we found that the effect is not only due to the changing of the anisotropy of Ce atom as generally believed. Instead, the decrease of MAE is a collective effect that anisotropy contributions from transition metal sites are also changed with N doping.

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