

Insights into anomalous magnetic hyperfine field at Ce impurity in LaMn_2X_2 (X=Si, Ge): a study from first principles calculations

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The LaMn_2X_2 (X=Si, Ge) intermetallic compounds doped with cerium exhibit the interesting physical effects that are typical of the $\text{RE}\text{Mn}_2\text{X}_2$ (RE=rare earth) series (such as magnetocaloric, superconductivity) or are originated from cerium in specific electronic environment (e.g. Kondo, intermediate valence, strongly correlated electron). Recently, the magnetic hyperfine field (*mhf*) at ^{140}Ce -doped $\text{LaMn}_2(\text{Si}_{(1-x)}\text{Ge}_x)_2$ was determined by perturbed gamma-gamma angular correlation spectroscopy. The ^{140}Ce *mhf* follow the host magnetization in LaMn_2Si_2 , while in $\text{LaMn}_2(\text{Si}_{(1-x)}\text{Ge}_x)_2$ (with $x = 0.2$ up to 1), it has anomalous behaviour, which was associated with $4f$ cerium *mhf* contribution. In this work, first principles band structure simulations were used to improve the understanding of the distance role (generated by interchange of Si and Ge) on *mhf* cerium contribution.