Insights into anomalous magnetic hyperfine field at Ce impurity in LaMn$_2$X$_2$ (X=Si, Ge): a study from first principles calculations

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The LaMn$_2$X$_2$ (X=Si, Ge) intermetallic compounds doped with cerium exhibit the interesting physical effects that are typical of the REMn$_2$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 LaMn$_2$(Si$_{1-x}$Ge$_x$)$_2$ was determined by perturbed gamma-gamma angular correlation spectroscopy. The $^{140}$Ce $mhf$ follow the host magnetization in LaMn$_2$Si$_2$, while in LaMn$_2$(Si$_{1-x}$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.