# Ferromagnetism in $CeRh_6Ge_4$: A DFT+DMFT study

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$CeRh_6Ge_4$ is a cerium-based compound that exhibits a ferromagnetic transition at $T_c = 2.5$ K. It has attracted significant attention due to the observation of a ferromagnetic quantum critical point under pressure, and associated non-Fermi-liquid behavior. Central to understanding these phenomena is the nature of Ce $4f$ electrons—whether they are localized or itinerant—and the mechanism stabilizing the ferromagnetic order. We investigate the ferromagnetic order in $CeRh_6Ge_4$, applying a recently developed method that succeeded in reproducing the quadrupolar ordering in a prototypical material, $CeB_6$ [1].

We employ a combination of density functional theory (DFT) and dynamical mean-field theory (DMFT) to investigate the magnetic properties of $CeRh_6Ge_4$. We begin with DFT calculations assuming itinerant $4f$ electrons, then incorporate strong local Coulomb interactions through DMFT, yielding localized $4f$ electrons. These calculations were done using the open-source software `DCore` [2]. With the converged solution in DFT+DMFT, we calculate the momentum-dependent susceptibilities using the strong-coupling-limit (SCL) formula, which was derived by approximating the Bethe-Salpeter equation in the DMFT [3]. We used the FAT node of the system B to treat the system size (the division of the Brillouin zone) up to $24 \times 24 \times 42$.

The results for the momentum-dependent susceptibilities reveal that the nearest-neighbor exchange interaction along the $c$-axis forms ferromagnetic chains, while weaker and anisotropic interactions in the $ab$-plane align these chains [4]. The intersite interactions follow an RKKY-like decay and are spin-isotropic along the $c$-axis but spin-anisotropic within the plane. The calculated transition temperature $T_c \approx 3.2$ K is in reasonable agreement with experiment, though slightly overestimated due to mean-field nature of the DMFT.

This work successfully reproduces the ferromagnetic ground state of $CeRh_6Ge_4$ using a localized $4f$ electron model and elucidates the microscopic origin of the magnetic ordering via intersite exchange interactions. It provides compelling theoretical evidence for the localized nature of $4f$ electrons at ambient pressure and a new insight of weakly interacting ferromgnetic chains. These findings establish a fundamental basis for elucidating pressure-induced quantum criticality in $CeRh_6Ge_4$.

## References

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