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A comparative study of CeCoIn5 and CeIrIn5 using DFT+DMFT
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— We present a comparative study of low temperature properties in heavy fermion materials CeCoIn5 and CeIrIn5 by means of the combination of density function theory and single-site dynamical mean-field theory. An efficient continuous-time quantum Monte-Carlo impurity solver in which charge fluctuations of $f^n \rightarrow f^{n\pm1}$ are treated as virtual processes without applying explicit Schrieffer-Wolff transformation is adopted in the simulation. The detailed evolutions of quasi-particle weight, Ce-4f density of states, momentum-resolved spectral functions and specific heat etc., are calculated in a temperature range $T \in [10, 100]$K. Upon decreasing temperature, both materials emerge heavily renormalized quasi-particle bands which are consistent with the ARPES experiments. Furthermore, we find that CeIrIn5, with a higher density states and a wider dispersion near Fermi level, is more itinerant than CeCoIn5.

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