Thermodynamics of the $\alpha$-$\gamma$ transition in cerium from first principles

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The Dynamical Mean Field Theory (DMFT) combined with density functional theory has been successful to describe strongly correlated materials [1]. However, the computation of the ground state properties requires a good accuracy from both the DFT and the DMFT side. We use thus a strong coupling Continuous Time Quantum Monte Carlo (CT-QMC) solver, which is fast and able to reach low temperatures, in combination with a projector augmented wave (PAW) DMFT implementation.

Extensive calculations using this implementation [2] allows us to carefully reassess the ground state properties and thermodynamics of the $\alpha$/$\gamma$ phase transition in Cerium at a large range of temperatures.

In particular, stochastic noise is small enough to avoid any ambiguity on the interpretation and the electronic entropy is included.

[1] G. Kotliar et al. Rev. Mod. Phys. 78, 865(2006)
[2] J. Bieder et al. Phys. Rev. B 89, 195132(2014)