Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Thermodynamics of the α-γ cerium phase transition from first principles JORDAN BIEDER, Univ of Tennessee, Knoxville, AMADON BERNARD, CEA, DAM, DIF, F-91297 Arpajon, France — The Dynamical Mean Field Theory (DMFT) combined with density functional theory in the local approximation has successfully described with a good accuracy strongly correlated materials. Thus, in this work, we focused on the $\alpha \rightleftharpoons \gamma$ cerium isostructural phase transition. However, in order to be predictive on ground state properties, a good accuracy must be obtained from the DFT and the DMFT side. For this purpose we use our self-consistent DFT+DMFT scheme in the PAW framework with our new implementation of the strong coupling Continuous-Time Quantum Monte Carlo (CT-QMC) solver to treat the impurity problem inside the DMFT. We start showing the need of charge self-consistency to study the ground state properties of cerium. Afterwards, we show the existence of two inflection points on the internal energy curves that disappear at very low temperature. Moreover, we compute the free energy to investigate the phase transition. Our DFT+DMFT scheme does not reproduce the phase transition but we do observe a softening of the bulk modulus which is a signature of the transition. Lastly, the inclusion of spin-orbit coupling is discussed. It is interpreted as a temperature renormalization. Indeed, our entropic stabilization at 800K is coherent with experiment at 400K.

Jordan Bieder
Univ of Tennessee, Knoxville

Date submitted: 18 Dec 2013 Electronic form version 1.4