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The isostructural $\alpha - \gamma$ phase transition in Cerium: a DFT+DMFT study. BERNARD AMADON, THOMAS APPLENCOURT, ALEXIS GEROSSIER, JORDAN BIEDER, CEA, DAM, DIF, F-91297 Arpajon, France, FABIEN BRUNEVAL, CEA, DEN, Service de Recherches de Mtallurgie Physique, F-91191 Gif-sur-Yvette, France, JULES DENIER, CEA, DAM, DIF, F-91297 Arpajon, France —

We present a study of the electronic structure and structural properties of the $\alpha - \gamma$ isostructural first order phase transition in cerium. Because of strong local electronic interactions due to 4f electrons, Density Functional Theory is not able to describe it. We thus use the combination of DFT and Dynamical Mean Field Theory, as implemented in ABINIT to understand and describe the transition:
Firstly, we use the constrained Random Phase Approximation to compute the effective interaction in cerium and discuss the validity of this approximation [1].
Secondly, we use this interaction to clarify the orbital mechanism of the transition: we thus discuss the validity of different models [2].
Thirdly, we compute the electronic free energy for the transition and discuss the role of entropy and spin orbit coupling [3,4].
Finally, we put in perspective our results with respect to recent calculations.

[1] B. Amadon, T. Applencourt, and F. Bruneval PRB 89, 125110 (2014)

[2] B. Amadon and A. Gerossier PRB 91, 161103(R) (2015)

[3] J. Bieder and B. Amadon PRB 89, 195132 (2014)

[4] B. Amadon, J. Denier and J. Bieder (unpublished)

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