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γ-α iso-structural Transition in Cerium[1] YONGXIN YAO, Ames laboratory–US DOE and Iowa state university, NICOLA LANATÀ, Rutgers University, CAI-ZHUANG WANG, Ames laboratory–US DOE and Iowa State University, JÖRG SCHMALIAN, Karlsruhe Institute of Technology, KRISTJAN HAULE, GABRIEL KOTLIAR, Rutgers University, KAI-MING HO, Ames laboratory–US DOE and Iowa State University — We present zero-temperature first-principle calculations of elemental cerium, and we compute its pressure-volume phase diagram within a theoretical framework able to describe simultaneously both the α and the γ phase. A surprising result revealed by our study is the presence of a clear signature of the transition at zero temperature, and that this signature can be observed if and only if the spin-orbit coupling is taken into account. Our calculations indicate that the transition line in the pressure-temperature phase diagram of this material has a low-T critical point at negative pressures, placed very close to zero temperature. This suggests that cerium is very close to being "quantum critical", in agreement with recent experiments.

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