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Orbital ordering and volume collapse in cerium[1] GÖKHAN ESIRGEN, University of Southern California, ANDREW K. MCMAHAN, Lawrence Livermore National Laboratory, RICHARD T. SCALETTAR, University of California, Davis — Realistic all-orbital many-body calculations are performed for cerium, covering a large volume range. 16-orbital cerium model Hamiltonians are obtained from the local-density approximation and solved using the fluctuation-exchange approximation. It is found that the thermodynamic behavior of cerium is coupled to orbital-ordering transitions of its f electrons. Different arrangements of f electrons occur for the α- and γ-cerium; moreover, metastable solutions also exist. In addition magnetic and spectral properties are analyzed.

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