

Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Phase Diagram and Electronic Structure of Praseodymium and Plutonium systems¹ YONG-XIN YAO, Ames Laboratory and Iowa State University, LANATA NICOLA, Rutgers University, CAI-ZHUANG WANG, Ames Laboratory and Iowa State University, GABRIEL KOTLIAR, Rutgers University, KAIMING HO, Ames Laboratory and Iowa State University — We apply a new implementation of LDA+Gutzwiller to calculate the zero-temperature phase diagram and electronic structure of Pr and Pu. Our study of Pr indicates that its pressure-induced volume-collapse transition would not occur without change of lattice structure — contrarily to Ce. Our study of Pu shows that the most important effect originating the differentiation between the equilibrium densities of its allotropes is the competition between the Peierls effect and the Madelung interaction. However, the proper treatment of electron correlation effects is crucial to reach good agreement with experiment. A similar interplay between correlation effects and bands structure is also displayed in Pr, and might emerge in even greater generality.

¹N.L. and G.K. supported by U.S. DOE BES under Grant No. DE-FG02-99ER45761. Research at Ames Lab supported by the U.S. DOE, Office of BES, DMSE, Ames Laboratory is operated for the U.S. DOE by Iowa State University under Contract No. DE-AC02-07CH11358.

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Date submitted: 14 Nov 2014

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