Abstract for an Invited Paper
for the MAR05 Meeting of
The American Physical Society

Correlation effects in the compressed rare earth metals[1]

ANDREW MCMAHAN, LLNL

A number of the trivalent rare earth metals (Ce, Pr, Gd, and Dy) are known to undergo electron-correlation driven phase transitions under pressure that are characterized by unusually large volume changes (5–15%). These "volume collapse" transitions demarcate regimes of different behavior with high-symmetry structures and local moments on the low-pressure (strongly correlated) side versus low-symmetry structures and screened moments on the high-pressure (more weakly correlated) side. Interestingly, Nd reaches this high-pressure regime without undergoing a significant collapse. This talk describes calculations using the local density approximation combined with dynamical mean field theory (LDA+DMFT) for Ce [1], Pr, and Nd, which seek insight into this behavior. Results for an assumed fcc structure suggest that the interesting correlation effects are pushed to higher pressures from Ce to Pr to Nd, and must compete there against successively stiffer underlying equations of state, which may contribute to the absence of the collapse in Nd. LDA estimates of the structure dependence of the energy appear to be smaller effects after these correlation contributions. Spin orbit plays an interesting role in that the lower Hubbard band remains exclusively j=5/2 under compression, whereas the quasiparticle weight is of mixed j=5/2, 7/2 character so that the pressure-induced transfer of spectral weight to the Fermi level effectively quenches the spin orbit. Collaborations with K. Held and R.T. Scalettar are gratefully acknowledged. [1] K. Held, A.K. McMahan, and R.T. Scalettar, Phys. Rev. Lett. **87**, 276404 (2001); A.K. McMahan, K. Held, and R.T. Scalettar, Phys. Rev. B 67, 075108 (2003).

[1]Work at LLNL was performed under the auspices of the U.S. Department of Energy by the University of California, Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.