Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

GW correlation effects on the quasiparticle energies of Np and Pu ATHANASIOS CHANTIS, ROBERT ALBERS, Theoretical Division, Los Alamos National Laboratory, AXEL SVANE, NIELS CHRISTENSEN, Department of Physics and Astronomy, University of Aarhus, MARK VAN SCHILFGAARDE, TAKAO KOTANI, School of Materials, Arizona State University — We present results for the electronic structure of plutonium and neptunium by using a recently developed quasiparticle self-consistent GW method (QSGW). The self-consistent GW quasiparticle energies are compared to those obtained within the Local Density Approximation (LDA) for several volumes of the unit cell. The goal of the calculations is to understand systematic trends in the effects of electronic correlations on the quasiparticle energy bands as a function of the localization of the f orbitals. We show that correlation effects narrow the f bands in two significantly different ways. Besides the expected narrowing of individual f bands (flatter dispersion), we find that an even more significant effect on the f bands is a decrease in the crystal-field splitting of the different bands. We discuss how these changes affect the topology of the Fermi surface and we demonstrate the importance of the quasiparticle self-consistency scheme in obtaining these results.

Athanasios Chantis
Theoretical Division, Los Alamos National Laboratory

Date submitted: 20 Nov 2008 Electronic form version 1.4