

Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

GW quasiparticle calculations with spin-orbit coupling for the light actinides¹ TOWFIQ AHMED, ROBERT C. ALBERS, Los Alamos National Laboratory, A.V. BALATSKY, Los Alamos National Laboratory; NORDITA, KTH Royal Institute of Technology and Stockholm University, Stockholm, Sweden, CHRISTOPH FRIEDRICH, Peter Grunberg Institut and Institute for Advanced Simulation, Germany, JIAN-XIN ZHU, Los Alamos National Laboratory — We report on the importance of GW self-energy corrections for the electronic structure of light actinides in the weak-to-intermediate coupling regime. Our study is based on calculations of the band structure and total density of states of Np, U, and Pu within a one-shot and spin-orbit coupling enabled formulation of the GW approximation within a full potential LAPWframework. We also present RPA screened effective Coulomb interactions for the f -electron orbitals for different lattice constants, and show that there is an increased contribution from electron-electron correlation in these systems for expanded lattices. We find a significant amount of electronic correlation in these highly localized electronic systems.

¹This work was supported by U.S. DOE at LANL under Contract No. DE-AC52-06NA25396, the LANL LDRD Program, and the Europe VR Program.

Towfiq Ahmed
Los Alamos National Laboratory

Date submitted: 15 Nov 2013

Electronic form version 1.4