Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

GW Study of Actinides: α-Uranium and δ-Plutonium R.C. ALBERS, A.N. CHANTIS, Los Alamos National Laboratory, M. VAN SCHILFGAARDE, Arizona State University, T. KOTANI, Arizona State Univeristy —
We have applied the recently developed Quasiparticle Self-Consistent GW (QSGW) method to α-U and δ-Pu. This is the first time that the f-orbital electron-electron interactions in actinides have been treated by a first-principles method that goes beyond the level of the generalized gradient approximation. We show that the QSGW approximation for U predicts a significant f-band narrowing when compared to GGA band-structure results. However, because of the low f-electron occupation number in U, ground-state properties are not significantly affected. This provides the first formal justification for the success of the LDA and GGA calculations in describing the gound-state properties of this material. For Pu we find that QSGW, like conventional band-structure calculations, predicts a static magnetic ground-state in contradiction with experiment. A non-magnetic solution is also presented. For δ-Pu we show that the QSGW approximation predicts even stronger band narrowing than for U. Because of this and a larger f-occupation, the ground state properties are affected much more significantly than for U. Overall, because of its better treatment of correlation, we suggest that the QSGW solution rather than GGA should be a better starting point for future Dynamical Mean Field Theory (DMFT) and other correlation methods.

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Date submitted: 23 Nov 2007 Electronic form version 1.4