Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Imaging electronic hot spots in the spectral function of the actinide $UCoGa_5$[1] MATTHIAS J. GRAF, TANMOY DAS, TOMASZ DURAKIEWICZ, JIAN-XIN ZHU, JOHN J. JOYCE, JOHN L. SARRAO, Los Alamos National Laboratory — We performed self-consistent GW-like calculations within the intermediate Coulomb-U coupling regime to investigate dynamic correlation effects in the intermetallic actinide $UCoGa_5$. This material is often used to contrast anomalous behavior in other U-115 and Pu-115 compounds, because it is presumed to be a conventional Fermi liquid that resembles a "vegetable." First-principles electronic structure calculations were used as input, combined with the spin-fluctuation exchange approximation, to compute self-consistently the many-body self-energy responsible for dynamic correlation effects. We validated theory by angle-resolved photoemission spectroscopy (ARPES). The occurrence of electronic hot spots in the spectral function, accompanied by kinks and abrupt breaks in the slope of the quasiparticle dispersion were detected both at low (130 meV) and high (1 eV) binding energies below the Fermi energy. In conclusion, we found that dynamic correlation anomalies are adequately described by coupling between itinerant fermions and spin fluctuations arising from the particle-hole continuum of the spin-orbit-split 5f states of uranium.

[1]We acknowledge computing allocations by NERSC under Contract No. DE-AC02-05CH11231.

Matthias J. Graf
Los Alamos National Laboratory

Date submitted: 11 Dec 2012 Electronic form version 1.4