

Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Electron Correlation and Transport Properties in Nuclear Fuel Materials¹ QUAN YIN, KRISTJAN HAULE, GABRIEL KOTLIAR, Rutgers University, SERGEY SAVRASOV, WARREN PICKETT, University of California, Davis — Using first principle LDA+DMFT method, we conduct a systematic study on the correlated electronic structures and transport properties of select actinide carbides, nitrides, and oxides, many of which are nuclear fuel materials. Our results capture the metal-insulator Mott transition within the studied systems, and the appearance of the Zhang-Rice state in uranium dioxide. More importantly, by understanding the physics underlying their transport properties, we suggest ways to improve the efficiency of currently used fuels.

¹This work is supported by the DOE Nuclear Energy University Program, contract No. 00088708.

Quan Yin
Rutgers University

Date submitted: 02 Nov 2010

Electronic form version 1.4