Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Phonon Spectra and Lattice Thermal Conductivity of UO2 and PuO2 QUAN YIN, SERGEY SAVRASOV, University of California, Davis — Electronic structure, phonon spectrum and lattice thermal conductivity of UO2 and PuO2 are studied using a combination of Density Functional Theory within Local Density Approximation and Dynamical Mean Field Theory (LDA+DMFT). UO2 and PuO2 are mixed oxides fuel (MOX) used in modern thermal reactors. Both oxides are Mott-insulators with strongly correlated 5f electrons, showing very similar electronic structures and phonon dispersions. The calculated phonon dispersion for UO2 is generally consistent with experiment and we give prediction for PuO2. Thermal conductivity is calculated based on the phonon dispersion. The phonon relaxation times are estimated in form of the Grüneisen constant derived from compressed volume phonon calculations.

Quan Yin
University of California, Davis

Date submitted: 15 Nov 2007 Electronic form version 1.4