Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

An LDA+U study of the photoemission spectra of ground state phase of americium and curium[1] MD ISLAM, ASOK RAY, University of Texas at Arlington, TX 76019 — We have investigated the photoemission spectra and other ground state properties such as equilibrium volume and bulk modulus of dhcp americium and the density of states and magnetic properties of dhcp curium using LDA+U method. Our calculations show that spin polarized americium is energetically favorable but spin degenerate configuration produces experimental quantities much better than that calculated using spin polarized configuration. The DOS calculated using LDA+U with both non-magnetic and spin polarized configurations is compared and the non-magnetic DOS is shown to be in good agreement with experimental photoemission spectra when U=4.5 eV. In spin polarized case, U is observed to increase the splitting between occupied and unoccupied bands by enhancing Stoner parameter. The results are shown to be in good agreement with that calculated using dynamical mean field theory for these two heavy actinides. For curium, exchange interaction appears to play the dominant role in its magnetic stability.

[1]The work is supported by the U. S. Dept. of Energy and the Welch Foundation.

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Date submitted: 22 Nov 2008 Electronic form version 1.4