

Abstract Submitted  
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**An *Ab Initio* Study of  $\text{PuO}_{2\pm 0.25}$ ,  $\text{UO}_{2\pm 0.25}$ , and  $\text{U}_{0.5}\text{Pu}_{0.5}\text{O}_{2\pm 0.25}$ <sup>1</sup>**

LI MA, ASOK RAY, University of Texas at Arlington — Hybrid density functional theory has been used to systematically study the electronic, geometric, and magnetic properties of strongly correlated materials  $\text{PuO}_{2\pm x}$ ,  $\text{UO}_{2\pm x}$ , and  $\text{U}_{0.5}\text{Pu}_{0.5}\text{O}_{2\pm x}$  with  $x=0.25$ . The calculations have been performed using the all-electron full-potential linearized augmented plane wave plus local orbitals basis (FP-L/APW+lo) method. Each compound has been studied at the ferromagnetic (FM) and anti-ferromagnetic (AFM) configurations with and without spin-orbit coupling (SOC) and *full* geometry optimizations. The optimized lattice constants, bulk moduli, and band gaps will be reported. Total energy calculations indicate that the ground states are AFM for all compounds studied here and the band gaps are typically higher than 1.0 eV, and characteristic of semiconductors. The total energy is lowered significantly and the band gaps increase with the inclusion of SOC. The chemical bonds between the actinide metals and oxygen atoms are primarily ionic in character.

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