First-Principles Study of Phase Stability, Electronic and Mechanical Properties of Plutonium Sub-oxides

P.S. Ghosh and A. Arya

Materials Science Division, Bhabha Atomic Research Centre, Trombay, Mumbai 400 085, India

Figure S1: Magnetic configurations of PuO$_2$ and Pu$_2$O$_3$. (a) 1-k AFM PuO$_2$ with the magnetic order along (0 0 1) lattice direction; (b) 1-k AFM Pu$_2$O$_3$ with the magnetic order along (0 0 1) lattice direction; (c) Regulski AFM Pu$_2$O$_3$ with four magnetic sublattices I, II, III and IV (d). In Fig. (a) and (b), the black and red balls designate Pu and O atoms, respectively. In Fig. (c), O atoms are removed for the sake of a clear indication of Pu magnetic order.