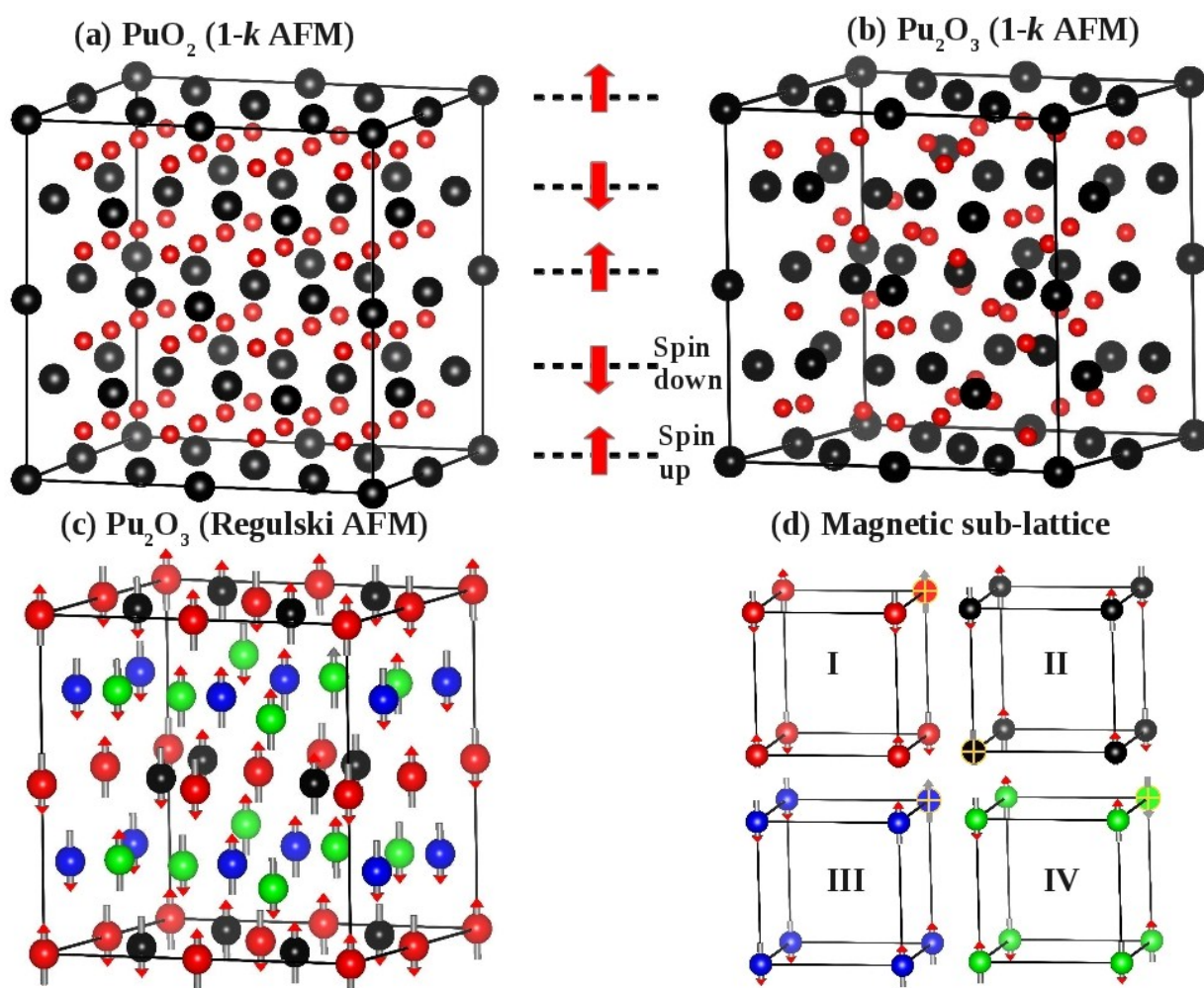


First-Principles Study of Phase Stability, Electronic and Mechanical Properties of Plutonium Sub-oxides

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Supplementary Information

Figure S1: Magnetic configurations of PuO_2 and Pu_2O_3 . (a) 1- k AFM PuO_2 with the magnetic order along (0 0 1) lattice direction; (b) 1- k AFM Pu_2O_3 with the magnetic order along (0 0 1) lattice direction; (c) Regulski AFM Pu_2O_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.