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Electronic, structural, and thermodynamic properties of mixed actinide dioxides (U, Pu, Am) O_2 from hybrid density functional theory[1]

LI MA, ASOK K. RAY, Physics Department, University of Texas at Arlington, TX 76019 — As a continuation of our studies of pure actinide metals using hybrid density functional theory,[2] we present here a systematic study of the electronic and geometric structure properties of mixed actinide dioxides, $U_{0.5}Pu_{0.5}O_2$, $U_{0.5}Am_{0.5}O_2$, $Pu_{0.5}Am_{0.5}$ O_2 and $U_{0.8}Pu_{0.2}O_2$. The fraction of exact Hartree-Fock exchange used was 40%. To investigate the effect of spin-orbit coupling on the ground state electronic and geometric structure properties, computations have been carried out at two theoretical levels, one at the scalar-relativistic level with no spin-orbit coupling and one at the fully relativistic level with spin-orbit coupling. Thermodynamic properties have been calculated by a coupling of first-principles calculation and lattice dynamics.

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[2]R. Atta-Fynn and A. K. Ray, Europhysics Letters, **85**, 27008-p1- p6 (2009); Chemical Physics Letters, **482**, 223-227 (2009).

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