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Electronic, structural, and thermodynamic properties of actinide dioxides[1] LI MA, RAYMOND ATTA-FYNN, 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 the actinide dioxides, UO_2, PuO_2 and AmO_2, using both density functional and hybrid density functional theories. For the hybrid density functionals, the fractions of exact Hartree-Fock exchange used were 25% and 40%. Each compound has been studied at the nonmagnetic, ferromagnetic and antiferromagnetic configurations, with and without spin-orbit coupling (SOC). The influence of SOC on the properties of the actinide dioxides will be discussed. Thermodynamic properties such as phonon dispersion curves, heat capacity, entropy, internal energy and free energy have been calculated by a coupling of first-principles calculations 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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