Abstract Submitted
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An *Ab Initio* Study of rare gases in uranium dioxide[1] LI MA, ASOK RAY, University of Texas at Arlington — Hybrid density functional theory has been used to study the stability and behavior of rare gases (He, Ne, Ar, Kr and Xe) in uranium dioxide. The calculations have been performed using the all-electron full-potential linearized augmented plane wave plus local orbitals basis (FP-L/APW+lo) method. Three insertion sites are considered: the octahedral interstitial position and the oxygen and uranium substitution sites. The defect formation energy, the optimized lattice constants and the volume variation induced by gaseous atom incorporation, and the electronic structure are studied for each rare gas in anti-ferromagnetic UO_2 phase without and with spin-orbit coupling (scalar vs. "full" relativistic). The results indicate that the lattice constants and formation energies increase with the increase of the radius of the rare gases. The octahedral interstitial position is the most favorable occupation site. All incorporation energies are found to be positive implying an exothermic process.

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Li Ma
University of Texas at Arlington

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