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DFT Energetics of Noble Gas Impurities and Schottky Defects in UO2 ALEXANDER THOMPSON, CHRIS WOLVERTON, Northwestern University Materials Science and Engineering, RADIATION DAMAGE IN NUCLEAR FUEL FOR ADVANCED BURNER REACTORS: MODELING AND EXPERIMENTAL VALIDATION TEAM — There is a strong need to better understand the mechanisms of nuclear fuel swelling in uranium dioxide (UO2) due to formation of fission product gases. Using density functional theory (DFT+U) calculations, we have explored the energetics of noble gases in UO2, Schottky defects (SD) in UO2, and the interaction between these defects. We find: (i) The noble gas atoms show a strong size dependence of the incorporation energy. (ii) The energetics of the SD in three different geometries shows that the preferred geometry is not simply driven by electrostatic effects. (iii) The energetics of each of the noble gas atoms incorporated in a SD show a strong favorable binding, due to strain relief. (iv) For Ar, Kr, and Xe, the binding energy of a noble gas impurity with the SD is larger than the energy required to form a SD, thereby providing an energetic pathway for the "spontaneous" formation of these defects. (v) From our calculations, we have constructed a simple model of the critical number of noble gas atoms required to form a bubble.

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