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**Defect Stability and Xe in UO2: Comparison between first-principles and classical potential calculations** ALEXANDER THOMPSON, DILPUNEET AIDHY, CHRIS WOLVERTON, Northwestern University, NERI-C 08-051 COLLABORATION — We have investigated defect stability and noble gas impurities in uranium dioxide (UO2) using a combination of Density Functional Theory and classical potential calculations. We consider a wide array of defects types, such as intrinsic vacancies and Schottky defects, as well as noble gas impurities such as Xe. We also consider the interaction between Xe and the vacancy clusters. We find Xe in an interstitial is a very high energy defect. It is energetically favorable to create a Schottky defect cluster for the Xe to incorporate into. We also examine transition states of point defect migration in UO2. We compare our results from DFT+U with several existing classical potentials, including potentials which are fit to first principles calculation. For our DFT+U calculations, we consider the problem of metastable orbital occupation that occurs in the DFT+U methodology.

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