Analysis of bulk properties and defect energetics in γ-U

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Uranium zirconium (U-Zr) alloys have a body centered cubic structure that shows a miscibility gap at the temperature of operation in sodium cooled fast nuclear reactors. The alloys exhibit a variation in composition under operation with zirconium atoms migrating up the temperature gradient. We examine several systems of U within a density functional theory framework utilizing the Vienna Ab-initio Simulation Package (VASP). We analyze our system with two separate generalized gradient approximations of the exchange-correlation. Bulk properties analyzed include the elastic modulus, lattice constant, and the Birch-Murnaghan equation of state for the γ-U phase. Defect parameters calculated include formation energies of vacancy, interstitial, and substitutional defects for the γ-U phase. These values are compared to computational and experimental results documented in the literature.