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An *Ab Initio* Study of Bulk γ-U and the (100) Surface[1] DAYLA MORRISON, ASOK RAY, University of Texas at Arlington — The properties of bcc γ-U have been studied using the formalisms of the generalized gradient approximation to density functional theory (GGA-DFT) and hybrid density functional theory. The computational formalism is the full potential linearized augmented plane wave method as implemented in the suite of software WIEN2k. Computations have been performed both without and with spin orbit coupling (SOC). Results indicate that GGA-DFT with SOC performs comparatively better in the description of the properties of γ-U, such as the non-magnetic ground state, lattice constant, and the bulk modulus. The predicted lattice constant and bulk modulus are 3.463 A and 114 GPa, respectively, to be compared with the experimental values of 3.467 A and 113 GPa, respectively. For the (100) surface, the monolayer exhibited significant contraction but the lattice constants tend to converge after 5 layers. Based on the results of the five layers, we predict the surface energy and the work function to be 1.46 J/m^2 and 3.24eV, respectively.

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