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Explaining the Properties of Plutonium with DFT[1] ACHYUTH MANOJ, University of Texas at Arlington, SARAH HERNANDEZ, Los Alamos National Laboratory, MUHAMMAD HUDA, University of Texas at Arlington — Plutonium, with atomic number 94, is a strongly correlated electron system, with the electronic configuration of Pu atom being Rn 5f6 7s2, making it a difficult material to perform theoretical calculations with. Plutonium is not a well understood element, and it shows anomalous properties, including but not limited to, showing six allotropic phases in its metallic state, with the ground state structure being a low symmetry monoclinic structure. With increased temperature, the structure changes to higher symmetry allotropes before melting. We use DFT (density functionals theory) implemented in the plane wave code VASP (Vienna Ab initio Simulation Package) to perform theoretical calculations on the allotropes of Plutonium to understand its properties. We use the GGA (generalized gradient approximation) functional in DFT to perform our calculations, and then include spin orbit coupling effects. We compare theoretical volume per atom to experimental values. Including spin orbit coupling effects gives us a better prediction for volume. Our DFT calculations predict that the lower temperature phases are nonmagnetic while the higher temperature phases are antiferromagnetic.

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