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Probing the Ground State of alpha-Plutonium with Density Functional Theory THOMAS BATES, RAYMOND ATTA-FYNN, Department of Physics, University of Texas at Arlington — Plutonium, Pu, has six different crystalline states as a function temperature. The room temperature phase, known as alpha-Plutonium (α-Pu), is a low-symmetry, monoclinic crystal, with distorted internal bonds. The α-Pu monoclinic crystal has several degrees of freedom so theoretical calculations on α-Pu often assume experimental lattice parameters and atomic positions to avoid optimizing the degrees of freedom. The key assumption in such calculations is that the experimental and theoretical lattice parameters and internal positions are similar. However, there is a possibility that differences exist between the theoretical ground structure and experimental structure. In this talk, the use of density functional theory (DFT) and several atomistic configurations of α-Pu to investigate the differences between the optimized theoretical structures and the experimental structure will be discussed.

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