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Stabilizing stored PuO₂ with addition of metal impurities¹

SHAFaq MOTEN, MUHAMMAD HUDA, University of Texas, Arlington — Plutonium oxides is of widespread significance due its application in nuclear fuels, space missions, as well as the long-termed storage of plutonium from spent fuel and nuclear weapons. The processes to refine and store plutonium bring many other elements in contact with the plutonium metal and thereby affect the chemistry of the plutonium. Pure plutonium metal corrodes to an oxide in air with the most stable form of this oxide is stoichiometric plutonium dioxide, PuO₂. Defects such as impurities and vacancies can form in the plutonium dioxide before, during and after the refining processes as well as during storage. An impurity defect manifests itself at the bottom of the conduction band and affects the band gap of the unit cell. Studying the interaction between transition metals and plutonium dioxide is critical for better, more efficient storage plans as well as gaining insights to provide a better response to potential threats of exposure to the environment. Our study explores the interaction of a few metals within the plutonium dioxide structure which have a likelihood of being exposed to the plutonium dioxide powder. Using Density Functional Theory, we calculated a substituted metal impurity in PuO₂ supercell. We repeated the calculations with an additional oxygen vacancy. Our results reveal interesting volume contraction of PuO₂ supercell when one plutonium atom is substituted with a metal atom.

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