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Plutonium hexaboride is a correlated topological insulator XIAOYU DENG, KRISTJAN HAULE, GABRIEL KOTLIAR, Department of Physics and Astronomy, Rutgers University, DEPARTMENT OF PHYSICS AND ASTRONOMY, RUTGERS UNIVERSITY TEAM — We predict that plutonium hexaboride (PuB_6) is a strongly correlated topological insulator, with Pu in an intermediate valence state of $Pu^{2.7+}$. Within the combination of dynamical mean field theory and density functional theory, we show that PuB_6 is an insulator in the bulk, with non-trivial Z_2 topological invariants. Its metallic surface states have large Fermi pocket at $\bar{X}$ point and the Dirac cones inside the bulk derived electronic states causing a large surface thermal conductivity. PB_6 has also a very high melting temperature therefore it has ideal solid state properties for a nuclear fuel material.

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