

Abstract Submitted
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Point defects in alpha and delta plutonium BABAK SADIGH, WILHELM WOLFER, Lawrence Livermore National Laboratory — We present first-principles calculations of the energetics of vacancies and interstitials in alpha and delta Pu. We perform calculations within spin-polarized density-functional theory. We analyze the lattice distortions around the point defects in terms of elastic relaxations as well as distortions induced by the change in the electronic structure of the host atoms due to the addition of the defect.

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