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Ab initio **equation-of-state and elastic properties of Pu metal and Pu-Ga alloys** PER SODERLIND, ALEX LANDA, Lawrence Livermore National Laboratory — We present results of *ab initio* calculations of equation-of-state and elastic properties for Pu metal and Pu-Ga alloys. For this we have employed density-functional theory (DFT) in conjunction with spin-orbit coupling and orbital polarization for the metal and coherent-potential approximation (CPA) for the alloys. All Pu systems benefit from spin polarization which is consistent with previous DFT studies of plutonium. We show that orbital correlations become more important proceeding from $\alpha \rightarrow \beta \rightarrow \gamma$ plutonium, thus suggesting increasing f-electron correlation (localization). For δ-Pu- Ga alloys we find that the system softens with larger Ga content, i.e., bulk modulus, elastic constants, and chemical bonding weakens with increasing Ga concentration. This inverse relationship is nearly linear and supported by measurements on polycrystal δ-Pu-Ga alloys. For Pu metal, our single-crystal results also relates reasonably with ultrasound data on polycrystal samples where available. The comparison is indirect but made possible by approximating the polycrystal with an isotropic (uniform strain) single crystal. This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

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