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Localization of 5f electrons and phase transitions in americium MICHEL PENICAUD, Commissariat a l'Energie Atomique — Density-functional electronic calculations have been used to investigate the high-pressure behavior of americium. The phase transitions calculated agree with the recent sequence obtained experimentally under pressure; double hexagonal close packed $\rightarrow$ face centered cubic $\rightarrow$ face centered orthorhombic $\rightarrow$ primitive orthorhombic. In the first three phases the 5f electrons are found localized, only in the fourth phase (Am IV) the 5f electrons are found delocalized. The localization of the 5f electrons is modeled by an anti-ferromagnetic configuration which has a lower energy than the ferromagnetic ones. In this study the complex crystal structures have been fully relaxed.

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