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On the interplay between spin polarization, orbital polarization and spin-orbit coupling in actinides from Pa to Cm[1] MD ISLAM, ASOK RAY, University of Texas at Arlington, TX 76019 — We present a systematic investigation of the effects of spin polarization, orbital polarization and spin-orbit coupling in six actinide elements, namely Pa, U, Np, Pu, Am and Cm using relativistic full-potential augmented plane wave with local orbital basis method. Our calculation shows that the $5f$ electrons in lighter actinides are itinerant with no magnetic effects. In heavier actinides, the $5f$ electrons are strongly correlated and quite sensitive to spin polarization, although the difference between FM and AFM energies tends to be very small. The orbital polarization has strongest effect in NM order and nearly vanishes for spin polarized calculations in almost all cases. The $5f$ electrons in α-Pu are close to being delocalized and their behavior is similar to that of lighter actinides. Among all the elements studied in this work, δ-Pu exhibits the most complex behavior. All forms of correlation effects are comparable in δ-Pu and significantly affect volume, bulk modulus and ground state energy.

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