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Valence Fluctuations and Quasiparticle Multiplets in Pu Chalcogenides and Pnictides CHUCK-HOU YEE, GABRIEL KOTLIAR, KRISTJAN HAULE, Rutgers University — The spectra of Pu chalcogenides and pnictides are computed with LDA+DMFT and interpreted with the aid of valence histograms and slave-boson calculations. We find the chalcogenides are mixed-valent ($n_f = 5.2$) materials with a strongly T-dependent low-energy density of states and a triplet of quasiparticle peaks below the Fermi level. Furthermore, we predict a doublet of reflected peaks above the Fermi level. In the pnictides, the raising of f^6 states relative to f^5 suppresses valence fluctuations, resulting in integral-valent ($n_f = 5.0$) local moment metals.

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