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The effect of core level crossing on the high-pressure equation of state of osmium JOHN WILLS, Los Alamos Natl Lab — The equation of state of the 5d transition metal osmium has been studied with a combination of experiment and theory at pressures up to 500 GPa. The experimental results show a c/a ratio increasing by approximately 1 percent over this pressure range and displaying anomalies at pressures near 180 GPa and near 400 GPa. We have use all-electron fully relativistic density functional theory (DFT) calculations to study the cold equation of state and structural parameters of osmium at pressures up to 500 GPa, using one LDA and two GGA functionals. The increase in the c/a ratio agrees well with experiment, and we find anomalies, although less extreme, near the experimentally observed pressures. We find that the high pressure anomaly coincides with the crossing and hybridization of the 4f(7/2) and 5p(3/2) semi-core levels. In this talk we discuss the theoretical results and methodology and the possible implication for the equations of state of the 5d transition and actinide metals.

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