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Core-Level Crossing and the High-Pressure Equation of State of Heavy Elements JOHN WILLS, Los Alamos Natl Lab — The structural properties of the *5d* transition metal osmium have recently been probed at static pressures up to $\sim$ 770 GPa [1]. In this study, anomalies in the *hcp* c/a ratio were found at pressures of in the vicinity of 150 GPa and 440 GPa. The anomaly at 150 GPa approximately coincides in pressure with an electron topological transition (ETT) observed in Density Functional Theory (DFT) band structure [1]. However, no ETT is observed at higher pressures. Instead, we find that the anomaly in the c/a ratio of osmium is correlated with the crossing of the $5p_{3/2}$ and $4f_{7/2}$ "core" levels, which at this pressure are found to have bandwidths $\sim$ .2-.3 Ry, in our DFT calculations. In this talk, I discuss the calculated structural properties and calculated equation of state of osmium and other heavy *5d* elements at pressures less than 1 TPa and the effect of core-level crossing on the equation of state and structural properties of these elements.

[1] Dubrovinsky, L., *et. al.*, in preparation.

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