Predicting Sommerfeld coefficients for heavy-fermion materials
MUNEHISA MATSUMOTO, SERGEY SAVRASOV, UC Davis, JUNYA OTSUKI, Tohoku University, Japan — From electronic-structure calculation standpoint we predict the appearance of heavy-fermion behavior for Cerium and Plutonium-based materials. Local-density approximation (LDA) combined with dynamical-mean field theory (DMFT) formulated for localized f-electrons gives an efficient realistic Kondo-lattice description [1] for the target materials, yielding a quasiparticle renormalization factor $z_c$ for conduction electrons. We invert the data to get the quasiparticle renormalization factor $z_f$ for f-electrons, and restore the effective total density of states to predict the Sommerfeld coefficient $\gamma$. Summarizing our data on an analogous “Doniach phase diagram” plotted for $z_c$, $z_f$, and $\gamma$, $\gamma$ is found to have a peak around the magnetic quantum critical point and Ce-115’s are found to have the largest $\gamma$’s among target materials.