Tuning the Eu valence in $EuPd_3B_x$: pressure versus valence electron count - a combined computational and experimental study

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Abstract

In a joint theoretical and experimental study we investigate the pressure dependence of the Eu valence in $EuPd_3B_x$ ($0 \leq x \leq 1$). Density functional band structure calculations are combined with x-ray absorption and x-ray diffraction measurements under hydrostatic pressures up to 30 GPa. It is observed that the heterogenous mixed-valence state of Eu in $EuPd_3B_x$ ($x \geq 0.2$) can be suppressed partially in this pressure range. From the complementary measurements we conclude that the valence change in $EuPd_3B_x$ is mainly driven by the number of additional valence electrons due to the insertion of boron, whereas the volume change is a secondary effect. A similar valence change of Eu in $Eu_{1-x}La_xPd_3$ is predicted for $x \geq 0.4$, in line with the suggested electron count scenario.