

First principles study of valence and structural transitions in rare earth compounds under pressure.

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The self-interaction corrected (SIC) local spin-density (LSD) approximation is used to study the sequence of structural and electronic transitions that occur in rare earth compounds (rare earth mono-tellurides and EuO) under pressure. It emerges that at ambient conditions all the rare earth tellurides (RTe) are stabilized in the NaCl (B1) structure. The corresponding rare earth valency is nominally trivalent (R^{3+}), with the exception of SmTe, EuTe, DyTe, TmTe, and YbTe, that are characterized by a divalent (R^{2+}) ion, corresponding to a fully localized f-electron configuration. Under pressure the CsCl (B2) structure becomes energetically favourable. Whilst the trivalent RTe undergo an isovalent structural transition, the divalent RTe are characterized by a succession of structural and valence transitions, the order of which is determined by the degree of f-electron localization. This interplay between structural and electronic degrees of freedom becomes even more noticeable in EuO. Here, starting from the Eu^{2+} ground state, an insulator to metal transition around 48 GPa leads to an valency increase in the B1 phase, followed at around 60 GPa by a structural transition to a B2 phase with an associated decrease in valency. This scenario is in line with the reentrant valence behaviour observed in recent pressure experiments.