# Systematic studies of electron-electron correlation effects in scandium-TM compounds

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**ABSTRACT**---Density functional theory calculations are carried out to explore electron-electron correlation effects in intermetallic compounds, scandium transition metals having 3d, 4d and 5d states. The calculations are carried out with the linearized augmented plane-wave plus local orbital (LAPW+lo) method. The exchange-correlation functional is treated by the LSDA, LSDA+U and LSDA+U. The correlation effects are evaluated for each compound by calculating the ratio of the on-site Hubbard parameter to the bandwidths (U/W) of the d-state of the compounds. Our results of this systematic study reveal that the electron-electron correlation effects decrease with the change of the transition metal from top to bottom in the same column of the periodic table, i.e., from 3d to 5d compounds.

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