Lanthanide contraction in $RENi_5$ (RE=La, Ce, Nd, Sm, Eu, Gd, Tb, Yb) compounds studied with band structure calculations

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FP-LAPW band structure calculations were performed for hexagonal $RENi_5$ (RE = rare earth) compounds in order to investigate reproducibility of lanthanide contraction by *ab initio* studies. The a and c parameters were optimised using a paraboloid fit, starting from the same initial values for all compounds studied. The trend in lattice parameters across the $RENi_5$ series obtained from the calculations was found to be in general agreement with experimental data. Comparison of results obtained by GGA and GGA+U calculations is presented for several double counting schemes.

9.7 cm

13.4 cm

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