

Band structure, magnetic and thermodynamic properties of RNi_5Sn (R=La, Ce, Nd and Pr) compounds.

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The electronic structure, magnetic and thermodynamic properties of RNi_5Sn (R=La,Ce,Nd,Pr) compounds are calculated by ab-initio FPLO method within the local density approximation (LSDA and GGA). The exchange correlation potentials are assumed in the form of PW'92 and PBE'96. The effect of electron correlations is included in LDA+U approximation. These compounds crystallize in the hexagonal crystal structure (space group No.194). In this work we present the magnetic properties, band structures and the topology of the Fermi surfaces of LaNi_5Sn , CeNi_5Sn , NdNi_5Sn and PrNi_5Sn compounds. The thermodynamic properties (bulk modulus, Debye temperature) are calculated in the Debye-Gruneisen model using the equation of states (EOS) in the form of Birch-Murnaghan, Poirier-Tarantola and Vinet.

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