# ELECTRONIC STRUCTURE AND MAGNETIC PROPERTIES OF $RNi_5Sn$ (R=Pr, Nd) COMPOUNDS

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Electronic structure and magnetic properties of $PrNi_5Sn$ and $NdNi_5Sn$ compounds are calculatied by ab-initio method. These compounds have $CeNi_5Sn$ type structure (space group P63/mc) and they are studied as hydrogen storage materials. We used full-potential local-orbital minimum-basis (FPLO) method within the local spin density approximation (LSDA). The band calculations were performed for two types of the exchange correlation potentials: Perdew and Wang (PW) and Perdew Burke Ernzerhof (PBE-GGA). Ab-initio calculations were performed for full-relativistic and scalar-relativistic (LSD+U) method. We present the band structure, local and total densities of states, the Fermi surfaces and theoretical XPS spectra for $PrNi_5Sn$ and $NdNi_5Sn$ compounds.The spin and orbital magnetic moments for both systems are calculated within the LSDA method.

9.7 cm

13.4 cm

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