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High pressure study of RNi intermetallics (R=Dy, Gd) POOJA RANA, UDAI PRATAP VERMA, School of Studies in Physics, Jiwaji University, Gwalior — The structural, electronic and magnetic properties of RNi's (R=Dy, Gd) have been analyzed using *ab-initio* full-potential linear augmented plane wave method within the density functional formalism. Spin polarized GGA+U approximations based on exchange-correlation energy optimization has been used for the calculation of total energy of the systems. Under compression, DyNi undergoes a first–order structural phase transformation from ambient FeB to CsCl phase at 18.4 GPa while GdNi transform its structure from CrB to CsCl phase at 3.73 GPa. The calculated magnetic moment for R^{3+} ions are obtained as 9.3 μB and 7 μB, respectively, in DyNi and GdNi. The results are closer to the experimental values (10 μB for Dy^{3+} and 7 μB for Gd^{3+}). Details related to structural, electronic and magnetic properties are reported, theoretically, for the first time for DyNi intermetallic compound. The equilibrium lattice constants are in good agreement with their experimental data. Our calculation shows that both the intermetallic compounds are metallic in nature.

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