Electronic topologocal changes in ferromagnetic $PrAl_2$

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The electronic structure of ferromagnetic $PrAl_2$ has been investigated by self-consistent tight binding linear muffin-tin orbital method (TB-LMTO) From the spin-polariszed calculation, it is found that $PrAl_2$ is having a magnetic moment of 2.34 bohr magneton which agrees well with the experimental result. It is found that the magnetic moment decreases under pressure. The band structure and density of states are plotted as a function of pressure As pressure increases the Density of states (DOS) intially decreases. At $V/Vo = 0.75$ compression corresponding to a pressure of 10.1 GPa, DOS begins (both spin up and down) increases first and then decrease. This may be due to appreance of a new piece of Fermi surface around the K-G direction. In addition, the bonding nature of this compound is explained from the density of states and charge density plots. The electronic specific heat coefficient, cohesive and formation energies are calculated and compared with the available literature.

9.7 cm

13.4 cm

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