# First principles study of the structural, elastic and electronic properties of Ti2InC and Ti2InN


## Abstract

The structural, elastic and electronic properties of $Ti_2InC$ and $Ti_2InN$ compounds have been calculated using the full-potential linear muffin-tin orbital (FP-LMTO) method. The exchange and correlation potential is treated by the local density approximation (LDA). The calculated ground state properties, including, lattice constants, internal parameters, bulk modulus and the pressure derivative of the bulk modulus are in reasonable agreement with the available data. The effect of pressure, up to 40 GPa, on the lattice constants and the internal parameters is also investigated. Using the total energy-strain technique, we have determined the elastic constants $C_{ij}$, which have not been measured yet. The band structure and the density of states (DOS) show that both materials have a metallic character and $Ti_2InN$ is more conducting than $Ti_2InC$. The analysis of the site and momentum projected densities shows that the bonding is achieved through a hybridization of Ti-atom d states with C (N)-atom p states. Otherwise, it has been shown that Ti–C and Ti–N bonds are stronger than Ti–In bonds.