ABSTRACT:

Transition metal carbide, nitride, carbonatite have attracted much attention due to their outstanding properties. The structural, electronic, optical, elastic, and thermal properties of transition metal carbide X_nC (X = V, Nb, Mo, $n = 2$) are investigated in the framework of Density Functional Theory (DFT). These calculations are based on first principle technique within Full Potential Linearized Augmented Plane Wave (FPLAPW) method. For the exchange correlation, Local Density Approximation (LDA) and Generalized Gradient Approximation (GGA) are employed which are embedded in Wien2k-code. The calculated structural, electronic, optical, and thermal parameters are found in good agreement with the available literature. Furthermore, the structures of the compounds are found orthorhombic having space group (60_Pbcn) and possess metallic nature. The associated quantities such as the dielectric function, energy loss function, reflectivity and absorption spectra are also evaluated by ab-initio calculations. Elastic properties of X_nC (such as C_{11}, C_{22}, C_{33}, C_{44}, C_{55}, C_{66}, C_{12}, C_{13}, C_{23}, Young's, bulk, and shear moduli) are evaluated at a pressure range of 0 to 100 GPa. By increasing pressure, transition metal carbides are found moving from ductile ($B/G > 1.75$) to brittle ($B/G < 1.75$) nature as per Pugh`s rule. The thermoelectric properties were calculated by solving the Boltzmann transport equation which revealed that (Mo_2C) shows a good electrical behaviour as compared with (Nb_2C) and (V_2C).