SUMMARY AND CONCLUSION

The conclusion of the AB INITIO results reported in this thesis is summarized in this section. The thesis entitled “AB INITIO STUDY ON STRUCTURAL CHANGES AND PHASE STABILITY OF SOME TRANSITION METALS UNDER PRESSURE” comprises the work done on the twelve transition metals from four different groups IVb, Vb, VIII and Ib in the periodic table.

i) Ti(Titanium), Zr(Zirconium) and Hf(Hafnium) – Group IVb

ii) V(Vanadium), Nb(Niobium) and Ta(Tantalum) – Group Vb

iii) Ni(Nickel), Pd(Palladium) and Pt(Platinum) – Group VIII

iv) Cu(Copper), Ag(Silver) and Au(Gold) – Group Ib

The entire thesis is organized in seven chapters. The results are

(1). We have investigated the pressure dependent band structure, density of states, structural phase transition and superconductivity of Titanium, Zirconium, Hafnium, Vanadium, Niobium, Tantalum, Nickel, Palladium, Platinum, Copper, Silver and Gold using FP-LMTO method.

(2). The total energies of Titanium, Zirconium, Hafnium, Vanadium, Niobium, Tantalum, Nickel, Palladium, Platinum, Copper, Silver and Gold are computed and the results are used to study the structural phase transition and superconductivity under pressure.

(3). In Titanium, we could find a phase transformation sequence of $\alpha$ (hcp) $\rightarrow$ $\omega$ (hexagonal) $\rightarrow$ $\gamma$ (distorted hcp) $\rightarrow$ $\beta$ (bcc) under pressure.
(4). From our analysis we predict a distorted bcc phase which is not stable at any high pressures.

(5). At normal pressure the hardness of Ti is in the following order: \(\omega\) - Ti > hcp - Ti > bcc - Ti > \(\gamma\)-Ti.

(6). When the pressure is increased, it is predicted that, \(T_c\) increases and reaches a maximum value thereafter \(T_c\) starts to decrease. The highest value of \(T_c(P)\) estimated is 5.043 K for hcp - Ti, 4.538 K for \(\omega\) - Ti and 4.85 K for bcc - Ti.

(7). From this, it is inferred that the maximum value of \(T_c(P)\) is rather insensitive to the crystal structure of Ti.

(8). The structural phase transition from hcp to bcc is found to occur at 0.32 Mbar for Zirconium and 0.48Mbar for Hafnium.

(9). At normal pressure the \(T_c\) is 0.53 K for Zirconium and 0.1254 K for Hafnium. This is in agreement with the experimental observation of 0.55 K for Zirconium and 0.12 K for Hafnium.

(10). The increase of \(T_c\) in bcc-Zr at 0.32 Mbar (5.807 K) and bcc-Hf is due to the softening of phonon modes which arises because of lattice softening induced by \(s \rightarrow d\) transition.

(11). We have investigated the pressure dependent band structure, density of states, structural phase transition and superconductivity of Vanadium, Niobium and Tantalum using FP-LMTO method.

(12). In Vanadium, Niobium and Tantalum, we could find a phase transformation sequence of bcc \(\rightarrow\) fcc under pressure. From our analysis we predict
hexagonal closed packed, simple cubic and Diamond phases are not stable at any high pressures.

(13). We have analyzed the structural phase transition from bcc to fcc structure in Vanadium, Niobium and Tantalum at 1.24Mbar, 1.34 Mbar and 1.70 Mbar respectively.

(14). The phase transition pressure of Vanadium as 1.24 Mbar and the corresponding reduced volume $V/V_0$ as 0.7, the phase transition pressure of Niobium as 1.34 Mbar and the corresponding reduced volume $V/V_0$ as 0.68 and the phase transition pressure of Tantalum as 1.70 Mbar and the corresponding reduced volume $V/V_0$ as 0.65.

(15). When the pressure is increased, it is predicted that, $T_c$ increases and reaches a maximum value thereafter $T_c$ starts to decrease.

(16). In Vanadium, at normal pressure, the value of $T_c$ calculated is 5.975 K. This is in good agreement with the experimental observation of (5.3 K) Ishizuka et al.

(17). At 1.2 Mbar pressure the calculated value of $T_c$ is 18.25 K which is very close to the experimental value of 17.2 K at 1.2 Mbar pressure. The highest value of $T_c$ 20.99 K, is reached at 1.393 Mbar pressure with a pressure coefficient of 10.78 K/Mbar, whereas the experimental pressure coefficient is 9.6 K/Mbar.

(18). In Niobium, at normal pressure, the value of $T_c$ calculated is 9.2425 K. This is in good agreement with the experimental observation of 9.5 K.

(19). The electron-phonon mass enhancement factor $\lambda$ at normal pressure is 0.7334, which is in agreement with the value of 0.74 reported by McMillan. At 1.25
Mbar pressure the calculated value of $T_c$ is 14.55 K which is very close to the experimental value of 14.8 K at 1.25 Mbar pressure. The highest value of $T_c$ 16.55 K, is reached at 2.47 Mbar pressure.

(20). In tantalum, at normal pressure, the value of $T_c$ calculated is 4.233 K. This is in good agreement with the experimental observation of 4.483 K. The electron-phonon mass enhancement factor $\lambda$ at normal pressure is 0.576, which is in agreement with the value of 0.574 reported by McMillan. At 1.39 Mbar pressure the calculated value of $T_c$ is 10.57 K which is very close to the experimental value of 10.8 K at 1.39 Mbar pressure. The highest value of $T_c$ 13.523 K, is reached at 2.667 Mbar pressure.

(21). We have analyzed the structural phase transition from fcc to hcp structure in nickel, Palladium and Platinum at 0.48 Mbar, 0.65 Mbar and 1.1 Mbar respectively.

(22). The phase transition pressure of nickel as 0.48 Mbar and the corresponding reduced volume $V/V_o$ as 0.85, the phase transition pressure of Palladium as 0.65 Mbar and the corresponding reduced volume $V/V_o$ as 0.83 and the phase transition pressure of Platinum as 1.1 Mbar and the corresponding reduced volume $V/V_o$ as 0.8.

(23). At normal pressure no superconducting behaviour. When the pressure is increased above 0.75 Mbar in Nickel, it is predicted that, the onset of superconductivity occurs and further increase of pressure $T_c$ increases and reaches a maximum value 1.46K.
(24). When the pressure is increased above 0.74 Mbar in Palladium, it is predicted that, the onset of superconductivity occurs and further increase of pressure $T_c$ increases and reaches a maximum value 8.864K.

(25). When the pressure is increased above 1.1 Mbar in Platinum, it is predicted that, the onset of superconductivity occurs and further increase of pressure $T_c$ increases and reaches a maximum value 0.664 K.

(26). We have analyzed the structural phase transition from fcc to hcp structure in Copper, Silver and Gold at 1.82 Mbar, 2.1 Mbar and 2.5 Mbar respectively.

(27). The phase transition pressure of Copper as 1.82 Mbar and the corresponding reduced volume $V/V_o$ as 0.65, the phase transition pressure of silver as 2.1 Mbar and the corresponding reduced volume $V/V_o$ as 0.62 and the phase transition pressure of Gold as 2.5 Mbar and the corresponding reduced volume $V/V_o$ as 0.65.

(28). At normal pressure no superconducting behaviour in Copper, Silver and Gold. When the pressure is increased above 2.83 Mbar in Copper, it is predicted that, the onset of superconductivity occurs and further increase of pressure $T_c$ increases and reaches a maximum value 2.248K.

(29). When the pressure is increased above 2.36 Mbar in Silver, it is predicted that, the onset of superconductivity occurs and further increase of pressure $T_c$ increases and reaches a maximum value 0.446K.

(30). When the pressure is increased above 4.185 Mbar in Gold, it is predicted that, the onset of superconductivity occurs and further increase of pressure $T_c$ increases and reaches a maximum value 1.879 K.
(31). So Nickel, Palladium, Platinum, Copper, Silver and Gold are comes under pressure-induced superconductors.

(32). The Tc-max values predicted for Ti and V lead to the conclusion that Tc-max is rather insensitive to the crystal structure.

(33). The factors which determine superconducting behaviour in materials are electron-phonon mass enhancement factor $\lambda$, and electron-electron interaction parameter $\mu^*$. Since the dependence of $Tc$ on electron-phonon enhancement factor $\lambda$ is more, these metals come under the class of electron-phonon-mediated superconductors.

(34). The normal and high pressure phases exhibit contrasting behaviour with respect to the high value of Tc (Tc-max). The above observations lead us to confirm that the highest Tc value depends more on the ground state structure rather than the high pressure structure.

(35). So if we retain the ground state structure under high pressure or create conditions equal to this, then one may achieve high Tc in these elements.

These results will be added as the new information to the Material Chemistry, Material Technology, Chemical and Material Engineering at normal and high pressure.