Band structure of ZnO (Wurtzite Structure)

ZnO is also known as zincite and has the wurtzite crystal structure. The wurtzite structure is an ABAB hexagonal close packing structure[1] as illustrated in **Figure 1**.

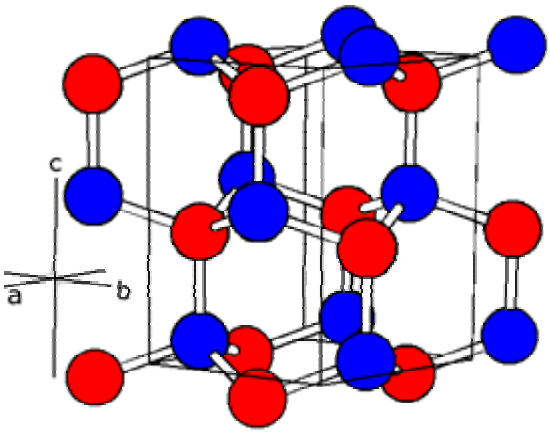

Figure 1: Wurtzite structure[1]

The band structure diagram of ZnO is given in **Figure 2.** The small bandgap (approx. 3eV) suggests that ZnO is semiconducting and this is verified by the literature.[2]

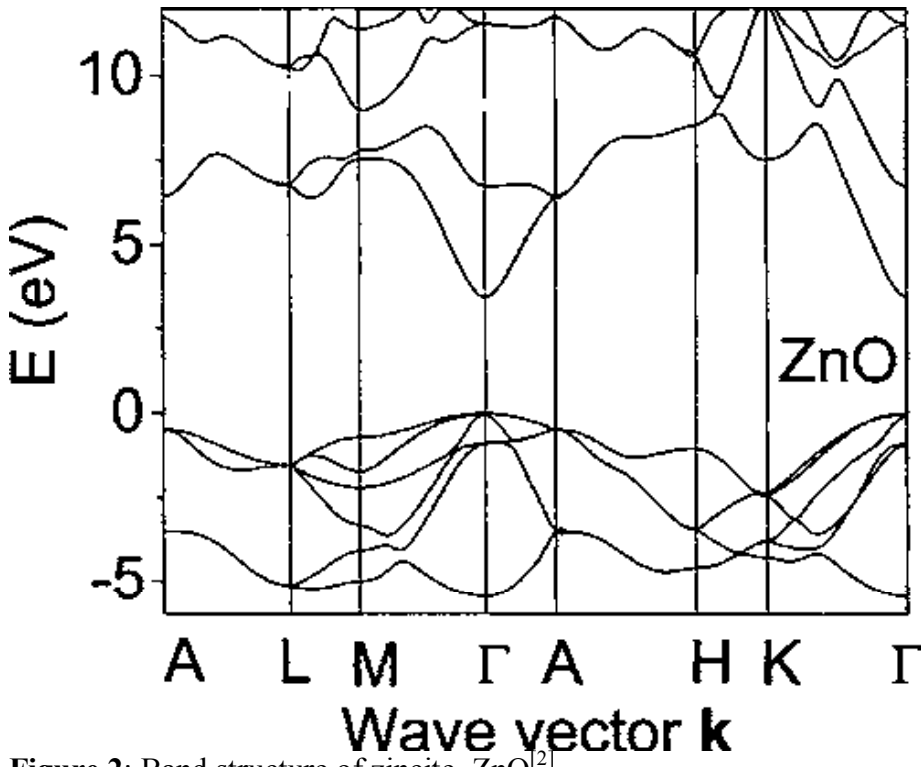

Figure 2: Band structure of zincite, ZnO[2]

There are a lot of low curvature bands which is characteristic of low mobilization of electrons and therefore localization in the d bands. Zn is a d-block metal so this type of behaviour is expected as the d orbitals are high energy and there electrons are involved in bonding interactions. These bands are mainly found in the valence bands of semiconductors. Ther are also high curvature bands typical for p_x orbitals of the O in the valence band. Bands with greater sp character are found in the conduction band and they are high curvature. These are molecular orbital interactions of the 3d orbital of Zn and 2s orbital of O.

[1] http://www.chemistry.ohio-state.edu/~woodward/ch754/struct/ZnO.htm
[2] W.J. Fan, X.B.Xia *et al*, *Journal of Applied Physics*, 2006, **99**, 013702