Abstract Of The Thesis

Scientists in this recent time are investing a lot of effort to study the physical and chemical properties of the materials. For advancement of industry, material science engineering has become a hot research topic in both theoretical and experimental fields. The vast variety of structural and physical properties exhibited by materials makes them promising for industrial applications. Material properties like structural, magnetic, optical properties primarily depend on the electrons. Study of electronic structure of materials thus forms an important area in condensed matter science. Advancement in technique like density functional theory (DFT), makes the theoretical study of electronic structure efficient. In this thesis, we will discuss about first principles DFT study of two distinct classes of materials. (i) crystalline transition metal oxide and (ii) materials at nano scale, primarily the clusters.

Crystalline transition metal oxides (TMO) have been in focus because of their tremendous application possibilities in industry. Charge, Spin, orbital ordering, complex phase transition in oxides make them site of many activities. Such classes of oxides have wide ranging applications in device engineering. On the other hand, rich varieties in the electronic properties among the nano-scale materials are noticed mainly because of the finite-size effect. Among different classes of nano scale materials, "clusters", a relatively small structure consisting of a few to few thousands of atoms, are one of the interesting class of nano-material because of their unique behaviour. Clusters have wide ranging applications in biomedical sciences, nano-catalysis. Large surface to volume ratio in clusters introduces many interesting properties. Electrons in such clusters produces discreet energy levels instead of forming continuous band feature. The abrupt change in electronic and structural properties of the nano-clusters compared to bulk materials has drawn the attention of many researchers during decades.

In this thesis, I report first-principle electronic structure results on nano-clusters as well as complex bulk materials such as A site ordered perovskite oxides.