

Abstract

This thesis entitled “**Density Functional Theory Approach towards Electronic Structures, Formation of High Valent Metal Species and Metal Mediated C-H/O-H Bond Activation**” is devoted to study on modeling structures, energetics of vanadium, chromium, manganese, iron, cobalt, nickel, and copper complexes containing amino ligands by using Density Functional Theory (DFT) methods. The C-H bond activation by metal-superoxo complexes has been investigated in detail using density functional theory (DFT). Mechanistic pathways studies for the catalytic reactions mediated by these transient species. Studies on different systems is presented in this thesis to (i) support/verify experimental findings, (ii) improve our understanding of the above-mentioned systems, and also (iii) make predictions to improve the efficiency, selectivity, and robustness of the existing catalysts. The results of this thesis are divided into four sections. In the first section, we have discussed electronic structures of iron TAML species, and their derivatives. In second section, we have studied the mechanistic study for selective C-H/O-H bond activation in the allylic system by using iron(V)-oxo TAML species. In the third section, we have studied the electronic structures of metal-superoxo species (where, M = V(III), Cr(III), Mn(III), Fe(III), and Co(III)) and also studied the effect of TMC-ring size on electronic structures and their comparative reactivity towards C-H bond activation. Our results reveal that ring size plays an important role in C-H bond activation. In the fourth section, we have discussed the formation of metal-oxo species with metal (Cr, Mn, Fe, Co, Ni, and Cu). Our findings suggest that the formation of earlier transition metal-oxo species have a smaller barrier than the late transition metal-oxo species.