Summary

This Thesis presents a quantum mechanical study of some F^+ laser centers in metal oxides SrO and CaO, Ab initio molecular electronic structure calculations have been carried out to examine (i) F^+ laser activity (ii) relaxed excited state orientational destruction of F^+ (iii) Glanser-Tompkins relation (iv) exciton (energy) transfer (v) the adsorptivity of the halogens (F, Cl and Br) at the defect free and defect containing surfaces. Ionic clusters of variable sizes were embedded in simulated coulumb fields that closely approximate the Madelung fields of the host surfaces, and commonly used methods (CIS and DFT) have been employed in the calculations.

The Thesis consists of three chapters scheduled as follow:

Chapter 1:

Presents a literature survey, short accounts on color center lasers and the theoretical methods employed in the calculations, namely, configuration interaction (CI-singles), and the density function theory (DFT).

Chapter 2:

F^+ laser activity and interaction of halogen atoms F, Cl and Br at the reduced oxygen coordination of SrO surface are investigated using the CIS and DFT methods of ab initio molecular electronic structure calculations in addition to several related properties such as the relaxed excited state orientational destruction, exciton (energy) transfer, relaxation and defect formation energies and the Glanser-Tompkins relation. The effects of F^+ center on the adsorption properties of the halogenatoms F, Cl Br and the role of covlent spin pairing are also examined.

Chapter 3:

F^+ laser activity and interaction of halogen atoms F, Cl and Br at the reduced surface coordination of CaO surface are investigated using the CIS and DFT methods in addition to investigating the very same properties examined for SrO. The differences between CaO and SrO surfaces in F^+ laser activites and interactions of halogens are demonstrated.