Summary

This thesis presents a quantum mechanical study of some laser centers in insulators. Ab initio molecular electronic structure calculations have been carried out to examine the F_A tunable laser activity at the low coordinated surface of KCl as well as F_2^+ tunable laser activity at the low coordinated surfaces of AgBr and LiH. Both the adsorptivity of halogen atoms on (KCl, LiH) and the donor-acceptor properties of O and O^- adsorbates at the flat surface of KCl crystal were examined. Photographic sensitization at the low coordinated surfaces of AgBr was also investigated. The examined (KCl, AgBr, LiH) clusters were embedded in simulated Coulomb fields that closely approximated the Maduling fields of the host crystal surfaces, and two commonly used methods, configuration interaction CI-singles and density functional theory DFT, have been employed in the calculations.

The thesis consists of five chapters:

Chapter 1:

Presents a literature survey, short accounts on color center lasers, photographic sensitization and computational techniques in addition to the theoretical models employed in the calculations namely, the configuration interaction CI-singles and density functional theory DFT.

Chapter 2:

In this chapter, Type I F_A (Rb^+,Cs^+) and II F_A (Li^+,Na^+) tunable laser activities, adsorptivity and donor-acceptor properties of O and O^- adsorbate at the

flat surface of KCl crystal were investigated using an embedded cluster model and ab initio methods of molecular electronic structure calculations. Ion clusters were embedded in a simulated Coulomb field that closely approximates the Madelung field of the host surface, and the nearest neighbor ions to the defect site were allowed to relax to equilibrium. Several related properties such as surface relaxation and defect formation energies and exciton band were investigated. In addition to the relative roles of energy gaps and covalent spin pairing.

Chapter 3:

In this chapter, an attempt has been made to examine F_A (Ga^+, In^+, Tl^+) tunable laser activity and adsorptivity of halogen atoms (F, Cl, Br, I, At) at the (001) surface of KCl crystal using an embedded cluster model and density functional theory DFT calculations with effective core potentials. The ion clusters were embedded in a simulated Coulomb field that closely approximates the Madelung field at the host surface. The nearest neighbor ions to the defect site were allowed to relax to equilibrium. The Glasner-Tompkins relation and the relaxed excited state orientational destruction of F_A were tested and the calculated adsorption energies were explained in terms of electron affinities, effective nuclear charges and electrostatic potentials.

Chapter 4:

In this chapter, The twofold potential of F_2^+ center at the low coordinated surfaces of AgBr thin films in providing tunable laser activity and photographic sensitization is investigated using ab initio methods of molecular electronic

structure calculations. The explicitly considered clusters were embedded in simulated Coulomb fields that closely approximate the Madelung fields of the host surfaces and the nearest neighbor ions to the F_2^+ defect sites were allowed to relax to equilibrium in each case. The RES orientational destruction of F_2^+ and the Glasner-Tompkins relation were examined. The developability of AgBr thin film, surface reduction and F_2^+ mobility were considered.

Chapter 5:

In this chapter, The twofold potential of F_2^+ color center at the low coordinated surfaces of LiH in providing tunable laser activity and adsorption properties for atomic halogens (F, Cl and Br) is examined using ab initio methods of molecular electronic structure calculations. LiH clusters of variable sizes were embedded in simulated Coulomb fields that closely approximate the Madelung fields of the host surfaces and the nearest neighbor ions to F_2^+ were allowed to relax to equilibrium in each case. The F_2^+ defect levels, the relaxation and defect formation energies, the F_2^+ orientational destruction were investigated and the results of the halogen-surface interactions were explained in terms of electrostatic potentials, band gaps and covalent spin pairing.