Abstract

The work in this thesis is a theoretical study of electronic structures of the F and other perturbed F-centers in ionic crystals of and structure. Our effort is concentrated on the calculation of the transition energies in absorption by using model potentials that are extracted from valid pseudopotentials. One of these is the BSG model which contains, in addition to the point ion potential, the ion size effect as fairly small corrections. Initially the problem of unperturbed center was investigated assuming a perfect lattice. The point ion theory was found reasonable as a starting point and was able to account for the general behavior of the F-centers but in a more accurate treatment the ion size correction need to be taken into account.

The perturbed F-center is characterized by the splitting of the first excited level (3-fold degenerate) into two levels; the first is non-degenerate and polarized along the defect axis, the second is 2-fold degenerate and polarized perpendicular to the defect axis. Numerically we adopted perturbation theory in the form of non-homogenous differential equation which was employed to predict these splittings.

The transition energies of FA, Z2+ and FH-center electron and in ionic crystals of and structure respectively, were found in good agreement with published theoretical results and available experimental data. Following the same procedure, the calculations were preformed on the center. This is a very involved defect because of the molecular ion in the and the latter was modeled as a point dipole in addition to being as a complete ion that resembles the ion. The results that were obtained are encouraging for pursuing further research on other similar centers like the FH (OH-), FH2 (OH-) centers.