ABSTRACT

In this thesis, we report the electronic and optical properties of III-V (III-N, III-P) and II-VI (BeX, MgX, CdX: X=O, S, Se, Te) semiconductors calculated using the first principle based full potential linearized augmented plane wave methods. Several exchange correlation functional extending from local to meta GGA type through semilocal (GGA) type were used for the calculations. The results for lattice constants of the above said materials show that general trend of underestimation by LDA and overestimation by PBE functional is confirmed for the studied materials also as observed in case of other classes of materials. It has been observed that LDA underestimate the lattice constants with MARE of 0.935%. On the other hand PBE overestimates with a MARE of 1.27%. WC and PBEsol give an improvement over the standard functional (LDA, PBE) for all classes of materials studied except in case of BeX where the results are of the same order as obtained with LDA. It is shown that no functional is good for all the materials studied. However, WC and PBEsol functional have been found to be better approximations in estimating the lattice constants and bulk modulus of III-V and II-VI binary compounds studied with smaller values of MARE (~ 0.3% and 6.5 %) for lattice constants and bulk modulus respectively. SCAN which is supposed to be the best functional in estimating the ground state properties of the solids shows a rather larger MARE (0.49%) for lattice constants of the materials studied, however it leads to almost same MARE (6.517%) for bulk modulus as that obtained with WC and PBEsol.

Next we performed the band gap calculations at optimized lattice constants obtained in with different approximations. From the results for the band gap, LDA and PBE have been found to underestimate the band gaps severely for all materials studied with a MARE of 48.57% and 47.66% respectively. In order to correct the band gap mBJ exhange potential in association with LDA correlation potential was used. mBJ has been found to improve the band gap over the standard DFT functionals with varying degrees of accuracy for different materials e.g. minimum MARE of 4.91% for III-P at PBE optimized lattice constants and maximum MARE of 23.91% for CdX materials with LDA optimized lattice parameters. mBJ band gaps at lattice constants optimized with different approximations are corrected to different degree. The results obtained show that there exists no general trend in this regard. From this study it has been observed that. it is not necessary to obtain the experimental band gap at lattice

constants closer to the experimental values. Concerning the improved parameterization of mBJ potential, no significant improvement over original parameters is observed. However, for III-N mBJSC provides the band gaps closer to the experimental values for III-N only while in all other classes of the material, mBJ with original parameters produces better agreement with the experimental band gaps. In the last the linear optical properties have been calculated for all the materials under study. In addition non linear second order susceptibility for some of non centrosymmetric materials has also been reported. The obtained results show a good agreement with earlier reported results.