Chapter 6

Future directions

In this thesis, the electronic structure of ZnSe and ZnO semiconductor quantum dots have been investigated. We employ density functional theory (DFT) to study the opto-magnetic properties of these materials. Based on our study, we report the optical absorption spectra of small, surface passivated ZnSe clusters. Doping of magnetic impurity, like Mn, alters the magic behaviour of these clusters. We report the discovery of a non-stoichiometric, magnetic, magic $\text{Zn}_{11}\text{MnSe}_{13}$ cluster, with a reduced magnetic moment of $3 \mu_B$. Doping of Mn in ZnO clusters, not only changes the magic behaviour, but further lowers the magnetic moment to $1 \mu_B$. These clusters can be thought of as nanocomposite, where a $\text{MnO}_x$ ($x = 1-4$) molecule is attached to the hollow cages of $(\text{ZnO})_n$ ($n = 12$ and $34$). Based on these results, several extensions to the current work can be initiated in near future:

- The importance of organic ligands in controlling the size, shape and growth of QDs is well known [46]. In our calculations, we have used fictitious, partially charged Hydrogen atoms for modeling the passivation in ZnSe clusters. However, with increasing computational power, it is now possible to directly attach the organic ligand to QDs. For instance, passivation has been directly modeled by attaching a trioctylphosphine molecule to CdS QDs [105].

- We have doped Mn in ZnSe and ZnO clusters. But a systematic study of doping $3d$ transition impurities like Mn, Cr, Ni etc, in all the II-VI combinations, viz., CdS, CdSe, CdTe, ZnS, ZnSe, ZnTe, ZnO, HgTe etc, is lacking. Our preliminary results show that except for CdSe, most of the combinations prefer anion rich, non-stoichiometric clusters when doped with Mn.

- In general, the Mn impurity in bulk and thin films of ZnO, attains a oxidation state of Mn$^{2+}$
due to 5 $\mu_B$ magnetic moment. However, recent experiments have observed mixed oxidation states of Mn, viz., Mn$^{3+}$ and Mn$^{4+}$ [31, 32]. Hence, a detailed first principles calculation of Mn doped in a thin film has to performed to understand these results.

- Investigation of optical properties of doped II-VI QDs would be a valuable addition to the current work, as the optical spectra can be directly compared with experimental observations.

- Colloidal core-shell QDs are attracting lot of attention due to their superior and tunable opto-magnetic properties. Studies based on cage-core structure of Zn$_{34}$Se$_{34}$ (Fig. 3.1w) can serve as a starting point for this study. For instance, the electronic structure of Zn$_{28}$Se$_{28}$ cage encapsulating a Cd$_6$Se$_6$ core, can be calculated. Doping and surface passivation can be also be initiated.

- Multi-scale modeling should be initiated to study the growth behaviour of large sized clusters.