

**Work done Report of
UGC-Minor Research Project on
Electronic Structure Studies of Small Clusters of ZnS and CdS**

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In this work, we have presented the results of our investigation into quantum confinement effects in ZnS and CdS clusters. These clusters have been most thoroughly investigated experimentally and there are reliable data to compare our theoretical results with. Furthermore, the bulk ZnS and CdS crystals exist in both zinc-blend and hexagonal crystal structures, because of which these clusters are ideal for investigating the size dependent crystal structure effect. The optical spectroscopy of these clusters is either at primitive stage or nonexistent at present, and we hope that our theoretical findings will focus experimental attention on these clusters.

We carried our pseudo potential band-structure calculations to investigate all these clusters. The significant findings of this study are as follows.

1. For ZnS and CdS clusters, our calculations have yielded exciton energies in excellent agreement with experiment over wide range of cluster sizes.
2. We also found that the shape, crystal structure and lattice constant of unit cell all have significant effect on the exciton energies.
3. The exciton energies of small and CdS clusters are in particular, sensitive to whether their crystal structure is zinc-blend or hexagonal, even though such a sensitivity is absent in large clusters.
4. The absorption spectra of these small clusters shift to red, instead of to the blue, with decreasing cluster size.
5. The Frank-Condon transition in small clusters, giving rise to the false origin in the absorption spectrum, exhibits the anomalous red shift with decreasing cluster size. On the other hand the non Frank-Condon transition, corresponding to the real origin of the absorption spectrum, does not show this effect.

All these findings, if confirmed by experiments, mean that clusters of different material compositions and crystal structure have widely differing optical properties and that the optical spectroscopy of small semiconductor cluster is dramatically different from those of large clusters and bulk crystals.