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Ph.D. Seminar
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Electronic and Optical Properties of Semiconductor Nanostructures

Semiconductors nanostructures have been shown to exhibit rich Physics, related to electronic, magnetic and optical properties. To understand the microscopic origins of these phenomena, first–principles calculations have and will continue to play a major role. In this thesis, first–principles studies are presented for various interesting semiconductors nanoclusters, with a view to understand how their size dependent properties will ultimately affect the various physical and chemical properties of these materials. So that new materials can be designed for integration into electronic, spintronic and optoelectronic devices.

We started our work with the ZnO semiconductor clusters. A systematic computational study of the electronic and optical properties of $(ZnO)_n$ clusters with n = 1 – 16, 24 and 36 using Time Dependent Density Functional Theory (TDDFT). The calculations bring out the role of dimensionality of clusters, multiple connectivity of Zn–O network and origin of blue–shift in the absorption spectra. Then we moved towards the carbon doped ZnO clusters to find impact of doping on host clusters. The study of ZnO clusters gives inspiration to locate another semiconductor material. The boron clusters are the suitable materials for this purpose. We critically analyze and discuss the optical properties and static polarizabilities of the boron clusters within the framework of the TDDFT. Similarly we also test the impact of doping with suitable materials in the boron. For that we choose alkali atoms such as lithium, sodium and potassium. The optical spectra are examined for pure and alkali doped boron. Our study reveals that the calculations of ZnO clusters help to design nanorods, nanowire and nanocomposites. Similarly the studied boron clusters help to built boron structures like boron ribbon, nanotubes and nanosheets etc.