QUANTUM MECHANICAL STUDY OF SEMICONDUCTING CLUSTERS

SUMMARY

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Chapter 1: Introduction

Matter is seen to be composed of atoms and molecules. Although individual particles have their characteristic properties, the bulk properties of given material also depends on its size and configuration. When number of constituent particles is sufficiently large, the properties saturate to an average value characteristic of given substance. However, the properties show reasonable variation from bulk counterpart when they aggregate to form a small system. What is more fascinating is that the variation in properties is abrupt if single atom is added to existing system comprising of a few to a few hundred number of atoms. Also the characteristic properties may fluctuate for various configurations for same number of atoms. Any material may be seen to be comprising of periodic arrangement of atoms, however little information exists regarding the manner in which atoms or molecules aggregate to form a bulk. It is assumed that a few to a few hundreds of atoms aggregate in a peculiar manner. Such aggregate is called a cluster and its properties differ drastically from bulk. The study of clusters has gained significance because they explain transition of properties from atomic to bulk regime. Clusters help understand the connection between the atomic and molecular physics on one hand, and condensed matter physics on the other. The study of semiconducting clusters assumes importance especially in semiconductor device fabrication industry. Cluster science grew up exponentially since later 1970s because of motivation to understand properties at reduced dimension and how one can gain expertise to manipulate them to desired criteria. The theoretical predictions play a significant role to design and model different materials as per requirements which are not always feasible via the experimental techniques as there is a high probability of reaction affinity of small size clusters. Thus, theoretical prediction of clusters and their characterization is a very hot topic of research in the present scenario. Since the properties of clusters depend on their composition, the properties can be fine-tuned resulting in novel optical and electronic capabilities.

ZnO is a wide band gap semiconductor which has drawn attention of the scientific and research community due to its application specially in the field of spintronics, transparent electronics and optoelectronics. Semiconductor like ZnO provides the possibility to the fabrication of devices which combine magnetic and optical effects and is suitable for spin LEDs, spin polarised solar cell, magneto-optical switches etc. CdS clusters find potential applications in material science because the electronic properties can be easily tuned. GaAs is one of the most important group III-V semiconductor that is suitable for use in high-efficiency solar cell. Very few contributions exist on Ge clusters. Only some workers produced some limited research on endohedral doping, ferromagnetism etc. It is an area which needs to be investigated thoroughly. GaN clusters form another most important class of semiconductor cluster after silicon and has revolutionised electronic industry.

In this work, quantum mechanical studies have been performed on Ga_xAs_x fullerene type micro-clusters, $(Ga_nN_n)_m$ micro-clusters, $Cd_xS_{x\pm4}$ fullerene like micro-clusters and phosphorus doped ZnO clusters using *ab initio* methods. Various parameters like binding energy, HOMO-LUMO gap, ionization potential, electron affinity, formation energy, polarizability etc. were calculated theoretically. To understand nature of formation of a bulk material of given substance, the effect of addition of atom to exisiting small cluster was studied. The study on isomer effect was also done to get information regarding the manner in which atoms aggregate to form clusters.The stability of structures was investigated for various configurations involving given number of atoms and electronic properties evaluated to analyze the suitability for applications in industry.

Chapter 2: Methodology

The structures were created using GaussView 5.0 which were fully optimized without any constraints. The optimized geometries were verified by frequency calculations through highly benchmarked B3LYP hybrid functionals that employ diffuse and polarization functions on clusters. Relativistic effective core potential (ECP) with double zeta basis set (LANL2DZ) were implemented in Gaussian 09 programme suite. Subsequently, electrical and optical properties were studied and structural stability was investigated. Gauss Sum 3.0 has been used for evaluation of density of states spectrum. The force component in each atom is calculated using conjugated gradient algorithm.

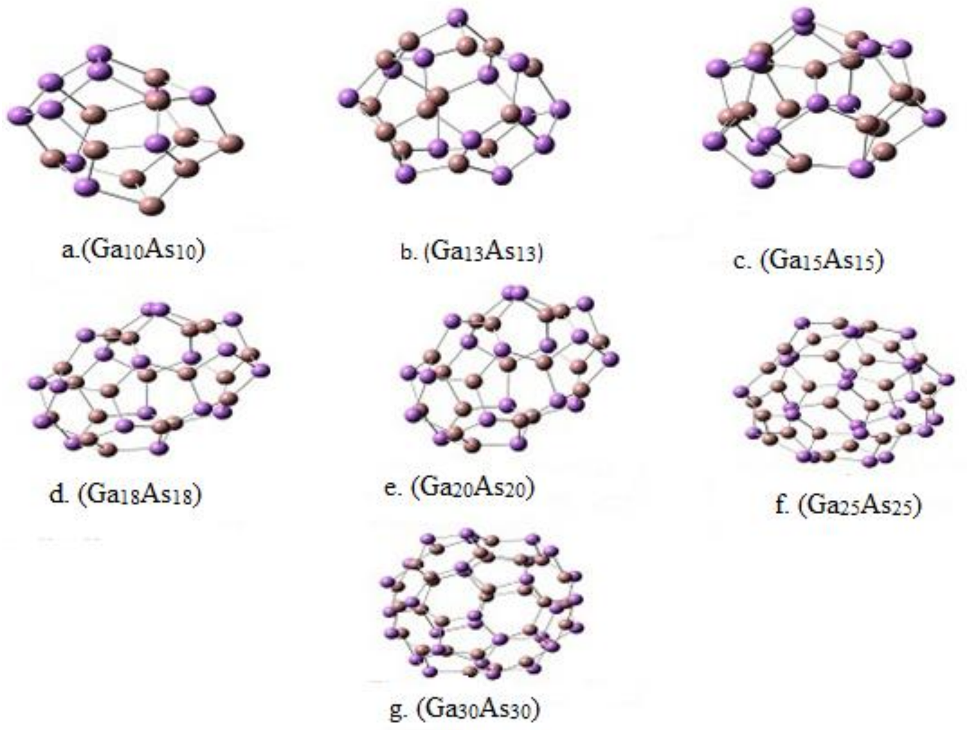
Chapter 3: Quantum mechanical study of Ga_xAs_x fullerene type micro-clustersfor x=10, 13, 15, 18, 20, 25 and 30 atoms

Low-dimensional semi-conducting material is of great interest to researchers in nano science. The dependence of electronic structure of the micro-cluster on its physical size gives rise to new physical, optical electronic chemical as well as magnetic properties. Investigation of clusters also enables to study the emergence of bulk crystalline properties from atomic or molecular scale. In order to obtain some desired property from a cluster, a detailed study about the properties of the cluster and its flexibility to control its size is required. The present day computational resources and techniques have enabled to model and investigate these clusters with ease and accuracy. Fullerenes have a special structure which consists only of pentagonal and hexagonal rings with hollow cage like structure and belongs to the class of micro-clusters. With all possible arrangement of collections of atom between these pentagon and hexagon many isomers can be constructed by varying the number of atoms. After the discovery of fullerene the interest has now shifted towards the search of new fullerene like structures formed by other elements or combination of different elements because fullerene type structures offer several unique properties that can be used in different applications like synthesis of nano-structured semiconducting magnets. III–V group semiconductor materials have been the focus of numerous experimentalists.Due to high electron mobility of III – V compounds such as GaAs these have the capability of replacing Si in the electronics industry. GaAs is a direct band gap semiconductor with band gap energy of ~ 1.43 eV. In the recent years several experimental and theoretical investigations of GaAs clusters have been done. It is expected that Gallium Arsenide cluster may exhibit different bonding characteristics than their bulk because of their strong anion-anion bonds. Investigations based on density functional theory (DFT) have been proven to be very useful for studying these type of micro-clusters. The present work is focused on the structures, as well as electronic properties of fullerene type Ga_xAs_x micro-clusters for x=10, 13, 15, 18, 20, 25 and 30 atoms.

The fullerene like Ga_xAs_x structures were generated using Gauss View 5.0. The optimization and study of the structures and characteristics of these clusters have been carried out by using the DFT with unrestricted B3LYP exchange-correlation potential as implemented in

Guassian 09 program. For describing the good geometrical and bonding feature for heavy atom, the basis set with effective core potential, LanL2DZ is used for Gallium (Ga) and Arsenic (As) atoms. The basis set LanL2DZ describes the outermost electrons of $3s^2$ $3p^6$ $4s^2$ $3d^{10}$ $4p^1$for Ga and As atoms. The interaction between core and valence electron was handled by Torullier-Martins norm conserving pseudo potential in their fully separable form and the pseudo potential also includes d orbitals in the valence configuration.

Optimized geometries were obtained without any symmetry constraints and continued until the force components on each atom are less than 0.01 eV/Å using a conjugated gradient algorithm. These optimized geometries were subsequently verified by frequency calculations. The presence of real or imaginary frequencies confirms the stability of structure.



a.($Ga_{10}As_{10}$)

b. ($Ga_{13}As_{13}$)

c. ($Ga_{15}As_{15}$)

d. ($Ga_{18}As_{18}$)

e. ($Ga_{20}As_{20}$)

f. ($Ga_{25}As_{25}$)

g. ($Ga_{30}As_{30}$)

Figure 1: The optimized structures of Ga_xAs_x micro-clusters for x= 10, 13, 15, 18, 20, 25 and 30.

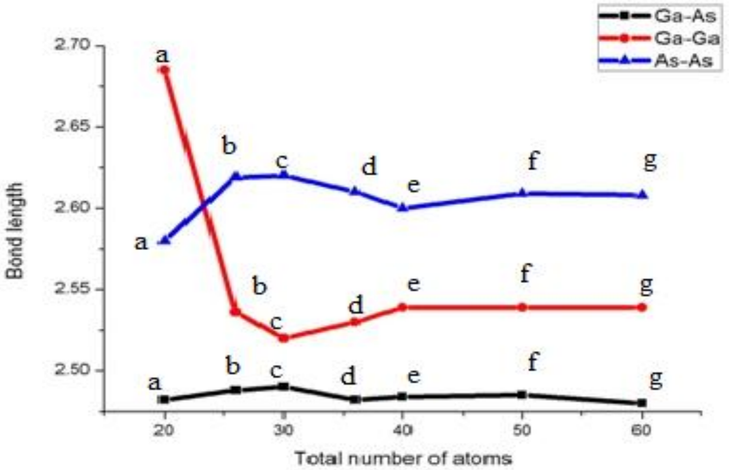
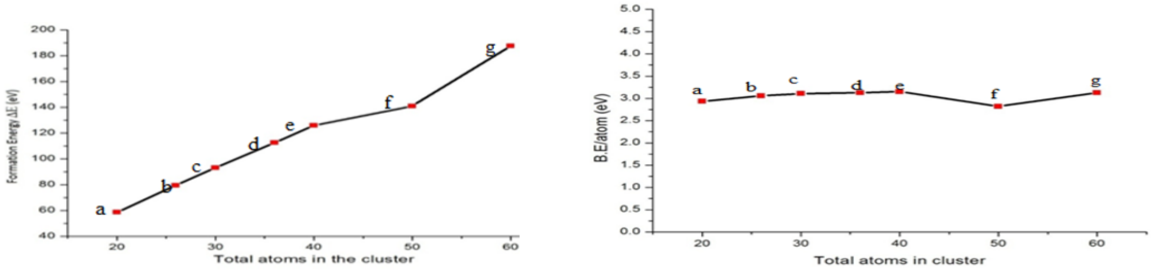
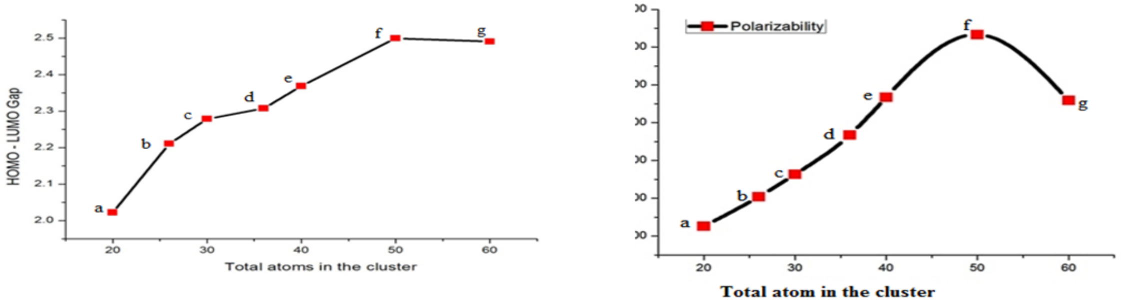


Figure 2: Variation of bond lengths in Å the Ga_xAs_x clusters for x = 10, 13, 15, 18, 20, 25 and 30.



Variation of formation energy in eV for Ga_xAs_x clusters for x = 10, 13, 15, 18, 20, 25 and 30.

The Variation of binding energy in eV for Ga_xAs_x clusters for x = 10, 13, 15, 18, 20, 25 and 30.



The variation of Homo-Lumo gap (E_g) in eV for Ga_xAs_x clusters for x = 10, 13, 15, 18, 20, 25 and 30.

The variation of polarizability in atomic unit for Ga_xAs_x clusters for x= 10, 13, 15, 18, 20, 25 and 30.

Figure 3: Variation of formation energy, Binding energy, HOMO-LUMO gap and Polarizability in the Ga_xAs_x clusters for x = 10, 13, 15, 18, 20, 25 and 30.

The energetic of possible reaction from reactants Ga and As to the products i.e. cluster depending on the stoichiometric of the clusters is obtained by the reaction

$$x(GaAs) \rightarrow Ga_xAs_x$$

The energy gap E_g is the difference of the highest occupied molecular orbital (HOMO) and energy of lowest unoccupied orbital (LUMO), this also represents the chemical stability of clusters. The optical activity of a cluster is related to its corresponding polarizabillity.

The electronic structure and optical properties of the Ga_xAs_x clusters for x= 10, 13, 15, 18, 20, 25 and 30 were studied using DFT method. The binding energy and HOMO-LUMO gap (E_g) confirms the stability of the clusters. The variation of polarizability, the optical activitywith increase in cluster size in the presented study suggests that $Ga_{25}As_{25}$ cluster has more optical activity in comparison with other studied clusters.

Chapter 4: Structural Stability and Electronic Properties of $(Ga_nN_n)_m$ Micro Cluster by using *Abinito* and tight-Binding Study

Gallium nitride (GaN) is an important semiconducting material, which has a broad range of potential applications for optoelectronics and high power electronic devices. Its high thermal conductivity also opened new routes in high-temperature and high –power electronic devices such as Metal Semiconductor Field Effect Transistor (MESFETs), High Electron Mobility Transistors (HEMTs) and heterojunction bipolar transistor (HBTs). Furthermore high Curie temperature and room temperature ferromagnetic nature has been predicted in GaN-doped with transition metal (MT).

To study the lowest–energy of $(Ga_nN_n)_x$ clusters, a number of possible structure isomers were generated. These structures were adopted from those previously proposed for the III-V semiconductor compound cluster such as BN, AlN.

Table 1: Illustrates the Binding energy, band gap and bond distance of $(Ga_2N_2)_m$Clusters.

Cluster	Binding energy/atom (eV)	Band gap (eV)	Bond distance (A^0)
$(Ga_2N_2)_1$	10.34	1.49	1.92
$(Ga_2N_2)_2$	10.81	0.84	1.91
$(Ga_2N_2)_3$	11.29	1.30	1.93
$(Ga_2N_2)_4$	11.48	1.33	1.92
$(Ga_2N_2)_5$	11.60	1.54	1.90
$(Ga_2N_2)_6$	11.61	2.43	1.91

Table 2: Shows the binding energy, band gap and bond distance of$(Ga_3N_3)_m$Clusters.

Cluster	Binding energy/atom (eV)	Band gap (eV)	Bond distance (A^0)
$(Ga_3N_3)_1$	10.92	2.11	1.87
$(Ga_3N_3)_2$	11.54	1.60	1.90
$(Ga_3N_3)_3$	11.83	2.12	1.92
$(Ga_3N_3)_4$	11.96	2.32	1.93
$(Ga_3N_3)_5$	12.05	2.39	1.92
$(Ga_3N_3)_6$	12.10	2.49	1.92

Table 3: Depicts the binding energy, band gap and bond distance of $(Ga_4N_4)_m$Clusters.

Atoms	Binding energy/atom (eV)	Band gap (eV)	Bond distance (A^0)
$(Ga_4N_4)_1$	11.15	2.65	1.77
$(Ga_4N_4)_2$	11.61	2.35	1.83
$(Ga_4N_4)_3$	11.83	2.52	1.91
$(Ga_4N_4)_4$	11.88	2.43	1.89
$(Ga_4N_4)_5$	12.00	2.69	1.89
$(Ga_4N_4)_6$	11.99	2.42	1.90

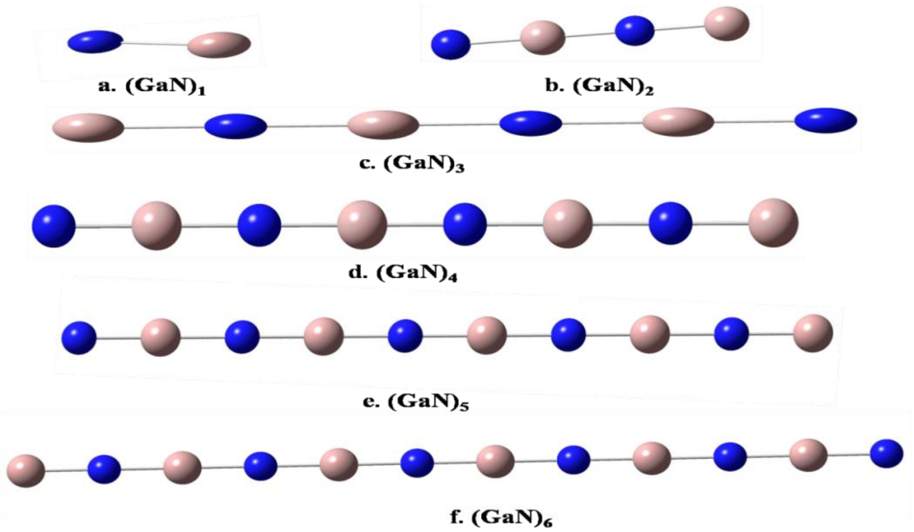
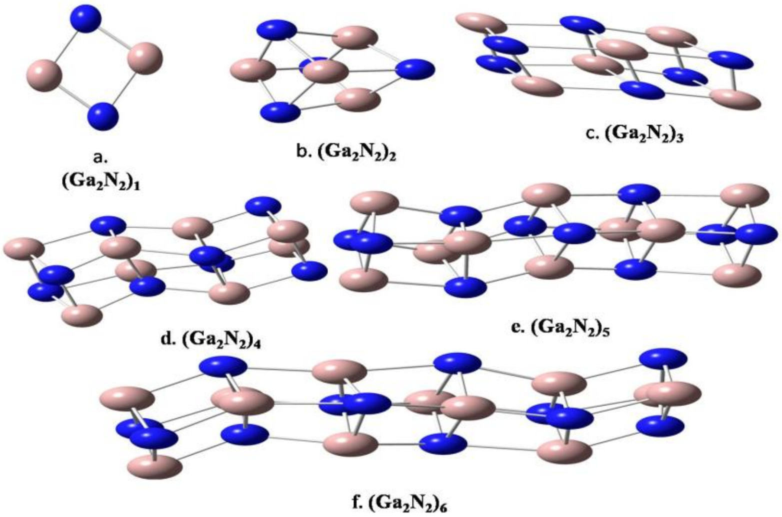


Figure 4 (a): Illustrates the Optimized structures of $(GaN)_m$micro cluster.



Figures 4(b): Illustrates the Optimized structures of $(Ga_2N_2)_m$cluster.

The binding energy per atom (BE) of a cluster is calculated using the formula:

$$\mathbf{BE} = \frac{\mathbf{nE(Ga)+nE(N)-E(GanNn)}}{2n}$$

where E (Ga), E (N), and E (Ga_nN_n) are total energy of a single Ga atom, a single N atom, and Ga_nN_n clusters, respectively and n is the number of Ga or N atoms. Similar calculations were extended to cluster to comprehend the first principle calculations on optimized Ga_nN_n nanowires with n=1-4.

First principle calculations on the various Ga_nN_n (n=1-4) clusters, were performed to obtain the stable isomers in each size range, which act as fundamental building blocks of condensed cluster or nano assemblies. The stable isomers of Ga_nN_n clusters from n=4 to 12 possess ring and cage (37) geometries respectively, which is quite comparable to earlier reports. With an understanding of stable isomers of Ga_nN_n with different geometries, condensed cluster of $(Ga_nN_n)_m$ are achieved by linear stacking of m up to 7 units of stable Ga_nN_n isomers (n=1-4). We also endeavor the condensation of the stable isomers of Ga_5N_5, but the important structural distortion was observed due to large aperture in the center of the rings.

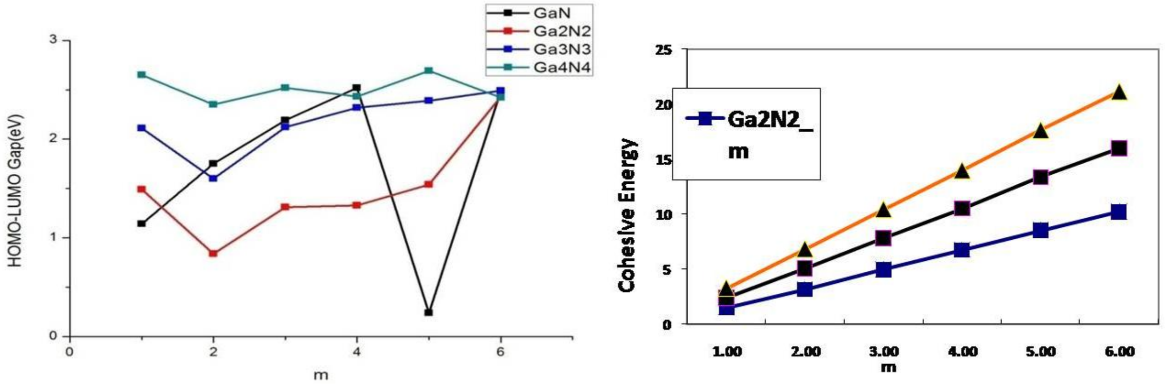


Figure 5: (a) Cohesive energy and (b) HOMO – LUMO Gap of $(Ga_nN_n\,)_m$ are shown. In the inset, BEs of $(Ga_nN_n\,)_m$ are shown for various n. The band gap shown in figure is less than the bad gap of bulk GaN, which is obtained from the calculation**.**

To study the structural stability of $(Ga_3N_3)_m$cluster the total and partial density of states (DOS) of the cluster with m=2,3 and 4 are studied and it is shown in Fig. 6. The DOS states are located in the energy range from -13.0 to -0.0 eV, while Ga (S P) states are distributed in the unoccupied region.These clusters can be understood on the structural stability of the molecular orbital theory.

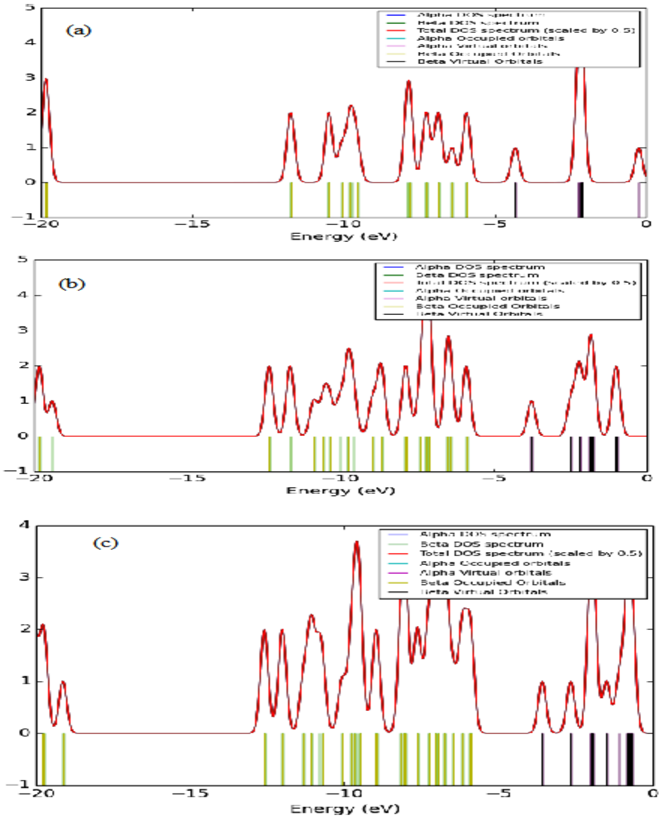


Figure 6: Total and partial DOS of $(Ga_3N_3)_m$ cluster with m=2(a), m=3(b), and m=4(c).

The fragmation energy per atom (FE) is calculated by using the formula:

$$FE = \frac{E[(Ga_3N_3)_n] + E[(Ga_3N_3)_m - n] - E[(Ga_3N_3)_m]}{6m}$$

The $(Ga_3N_3)_m$ may be divided into the following two pieces of a possible cluster: (1, m -1), (2, m-2), (3, m-3), (4, m-4). FE are calculated and shown in Figure 7(a).

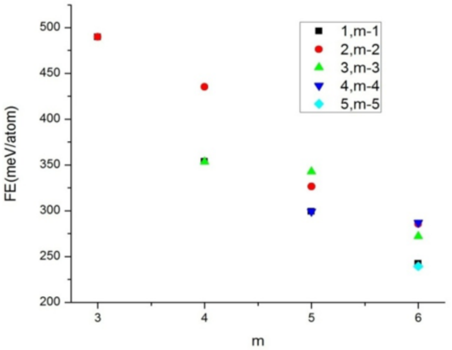


Figure 7(a): FE versus m of $(Ga_nN_n)_m$ of various possible fragments

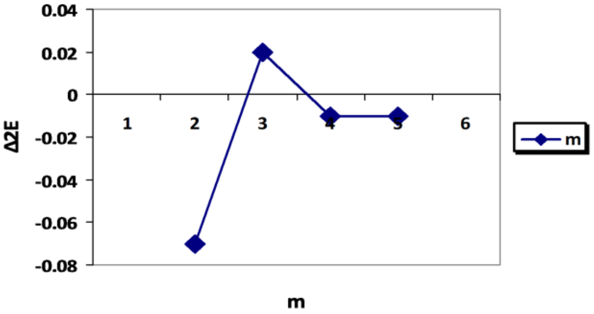


Figure 7(b): shows the second derivative of energy of $(Ga_3N_3)_m$ cluster with respect to m. The calculated value by using the formula $\Delta^2E = E(m+1) + E(m-1) - 2E(m)$

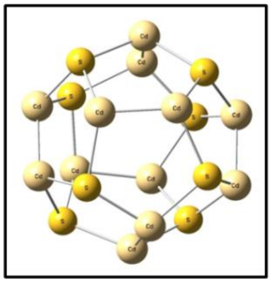
We condensed the second derivative of the total energy (Δ^2E) of the cluster and the cluster reveals about the structural stability and it is reported in Figure 7(b). Our calculations shows that the Δ^2E of $(Ga_3N_3)_3$ cluster shows the maximum value, and high structural stability of this cluster.

Chapter 5: Stability of CdxSx±4 fullerene like micro clusters predicted from ab initio DFT calculations

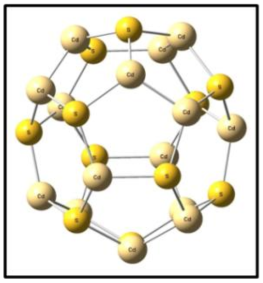
Several experiments have been performed from II-VI group in search of different semiconductor materials. II-VI group compounds have high electron mobility such as CdS, therefore the electronics industry may be inclined to replace Si. CdS is a direct band gap semiconductor with band gap energy of ~ 2.42 eV. In the recent years, several experimental and theoretical investigations of CdS clusters have been performed. These studies have enabled us to know more about the structural stability, reactivity and nature of bonding in these clusters. Thus the Cadmium Sulfide cluster may exhibit different bonding characteristics than their bulk counterpart which have the same bonding because of strong anion-anion interaction. The investigation of such clusters based on first principles methods has proven to be very useful for study.

The present work is based on the study of the structures, stabilities and electronic properties of $Cd_{x\pm4}S_{x\pm4}$ clusters possessing fullerene like hollow cage structures. Various possible structures of CdS fullerene depend upon the different composition of Cd and S which are governed by the formula $Cd_{x\pm4}S_{x\pm4}$, where x is the number of single type of atom present in the cluster. The value of x is varied and corresponding clusters so formed were studied.

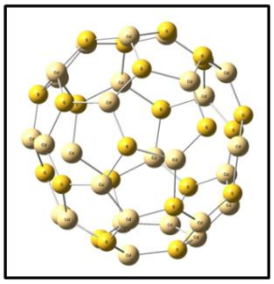
To determine the stability of Cadmium Sulfide fullerenes, cohesive energy, energy change in a model reaction, energy gap in electronic structure were considered. The structures with lower energies are energetically more favourable and stable than the systems with higher values. The Gaussian works in gaseous medium. So the lower energy of the cluster is utilised to decide which systems are chemically more stable. Smaller energy gap values are used for lower reactivity and thus contribute in the enhanced chemical stability.



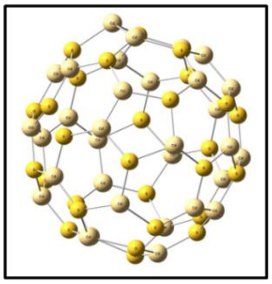
$Cd_{12}S_8$



$Cd_{15}S_{11}$



$Cd_{27}S_{23}$



$Cd_{32}S_{28}$

Figure 8: The Cd-rich Cd_xS_{x-4} non-IPR fullerenes. The shared edges of the pentagons are occupied by Cd atoms.

The optimized atomic structure of Cd-rich Cadmium Sulfide fullerenes with the formula of $Cd_{x+4}S_x$ are shown in Fig. 8 for $8 \leq x \leq 28$ where the light (creamish white) color represents the Cd atoms and yellow color represent the S atom. In each structure there are 12 pentagons and six edges are shared by adjacent pentagons. The Fig. 8 shows the isomers where Cd and S atoms could be placed to give the minimum number of homo-nuclear bonds. The common edges of adjacent pentagons consist of Cd-Cd bonds. However there are no homo-nuclear bonds.

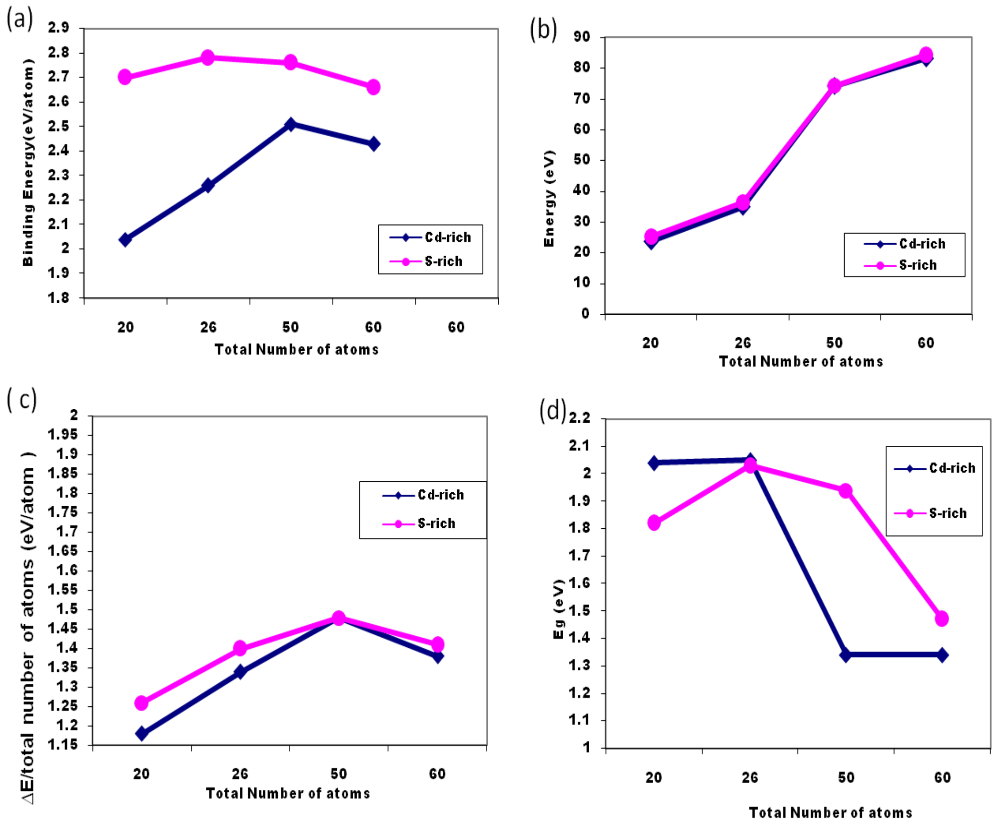


Figure 9: The energetics of Cd_xS_y non-IPR fullerenes in Cd-rich fullerenes (x=y+4) and in S-rich fullerenes (y= x+4) are shown. (a) Binding energy of the bulk Cd_xS_y fullerenes as a

function of the total number of atom. (b) The reaction energy during a synthesis of the fullerenes starting from bulk CdS and S_2 gas .the reaction energy per atom is shown in(c).

The atomic structure and stability of cadmium sulfide fullerenes ($Cd_xS_{x\pm4}$) is studied by using DFT method. It has been found that the hollow cadmium sulfide fullerenes are stable when the pentagon edges are shared which reduces the number of homo-nuclear bonds. The energetics and the energy gap in electronic structure as an indicators, for the stability of cadmium sulfide fullerenes is also investigated. The study predicts that these clusters are stable. The stability of the cluster increases when the number of homo-nuclear bonds in the cluster is less.

It is found that the binding energy of S-rich fullerene gets saturated when the size of the cluster is beyond 40 atoms.Therefore, the shared edges of adjacent pentagons, S atoms, bond angle are satisfied by only a small strain energy input. The bond lengths are not adequate to differentiate between the Cd-rich and S-rich fullerenes so this might be the possible reason for the lower total energy in S-rich fullerenes and that S-S bond are energetically more favorable than Cd-Cd bonds. This conclusion is in agreement with the findings that S atom clusters in small cadmium sulfide fullerenes clusters. (S- containing clusers) are more stable.

Chapter 6: Quantum chemical studies of Phosphorus doped ZnO cluster stability and electronic properties by using ab-inito method

Zinc oxide (ZnO) materials having n-type semiconductor are wide band gap 3.37 eV, which exhibits the Wurtzite structure. ZnO in its wurtzite lattice belongs to space group P63mc characterized by two subunits interconnected by Zn^{2+} and O^{2-} ions where zinc is surrounded by tetrahedral oxygen ions and vice versa.

The ZnO cluster due to its low ionization energy, ionic radius, easy availability, low toxicity and easy handlingis widely used in optoelectronic devices such as photo detectors, gas sensors, light emitting diodes, varistors, piezoelectric devices, batteries, fuel cells, photocellsas a catalyst.

The ZnO cluster has a potential applicationin solar energy conversion. ZnO has been recognized as a valuable optical material in the blue-UV region and has a large exciton binding energy. Very few works are reported based on the density functional theory (DFT) on ZnO clusters. DFT is preferable for application in materials science because it can handle bulk and structural calculations. One of the main advantages of DFT is to tailor the properties of materials without the feeding of the experimental data with a low computational cost relative to other method. To understand extremely efficient optoelectronic devices, it is mandatory to have high-quality single –crystalline p-type ZnO. Recently, enormous effort has been devoted in fabricating p-type ZnO via thin films using I and group V element as p-type dopants. There is a good scope to work on p-type ZnO nanowires (substituting of P and N) as very few works are reported in this field To study the structural stability of ZnO micro clusters, Phosphorus is added as an impurity. All Phosphorus doped Zinc Oxide ($Zn_xO_{x-1}P$) clusters for x=2-5 reported in this work are optimized by the B3LYP method as implemented in Gaussian 09 package.Various possible structures for each $Zn_xO_{x-1}P$ clusters are modelled and the stable structure is identified from the energetic.

The relevant parameters like energy, dipole moment values and point group of $Zn_xO_{x-1}P$ cluster for (x=2-5) are reported in Table 4

Table 4: Illustrate the various models of different cluster size.

Model	Cluster Size	Energy (Hartrees)	Dipole moment (Debye)	Point group
Linear	2	-3974.727373	2.01	Cs
	3	-5829.099738	2.03	Cs
	4	-7683.472522	2.15	C1
	5	-9537.843967	2.14	Cs
Ring	2	-3974.724212	0.28	Cs
	3	-5829.141279	0.29	Cs
	4	7683.537652	0.29	Cs
	5	-9537.922905	0.34	Cs
3D	3	-5829.141279	0.30	C1
	4	-7683.478453	1.05	C1
	5	-9537.903002	1.90	C1

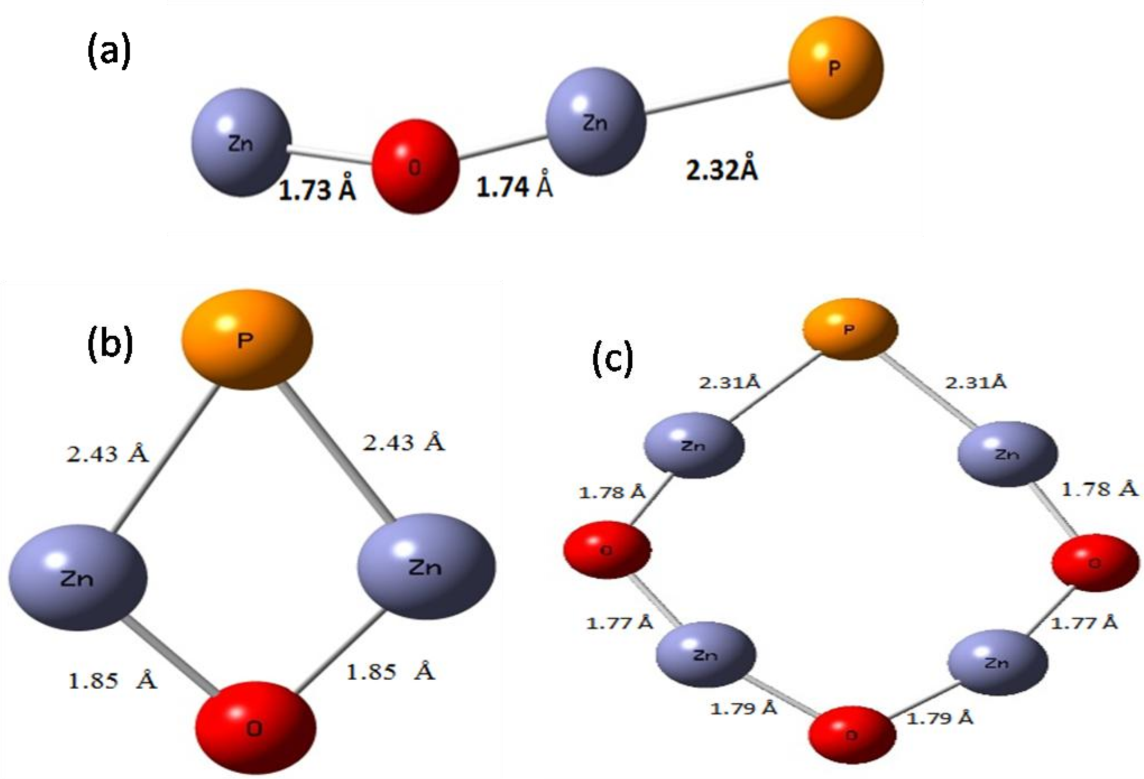


Figure 10: B3LYP/6-31G optimized geometrical structure of (a) Zn$_2$O$_1$P Linear Cluster (b)Zn$_2$O$_1$P Ring Cluster (c) Zn$_4$O$_3$P Ring Cluster

Table 5: Binding energy of $Zn_xO_{x-1}P$ (x=2-5) micro clusters

Cluster size	Linear (eV)	Ring (eV)	3D (eV)
2	2.73	2.71	-
3	3.30	3.49	3.50
4	3.59	3.81	3.61
5	3.76	3.96	3.90

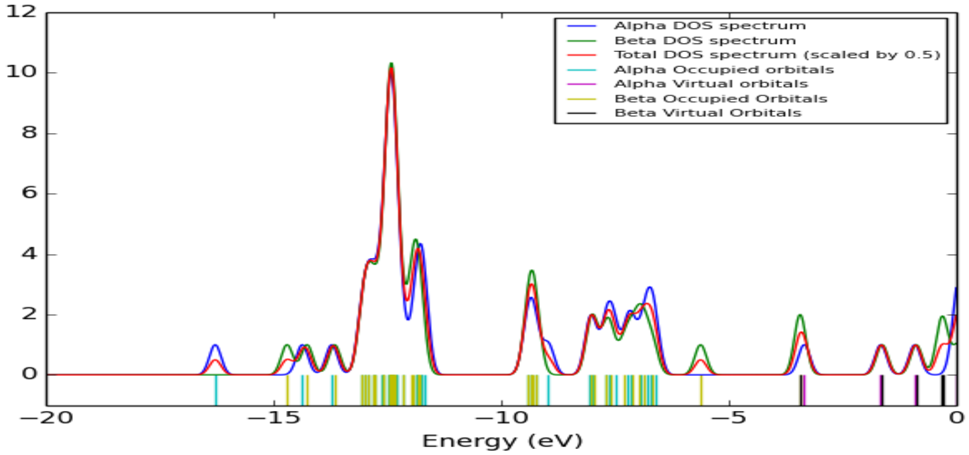


Figure 11(a): HOMO-LUMO, DOS spectrum of Zn_5O_4P micro cluster linear structure.

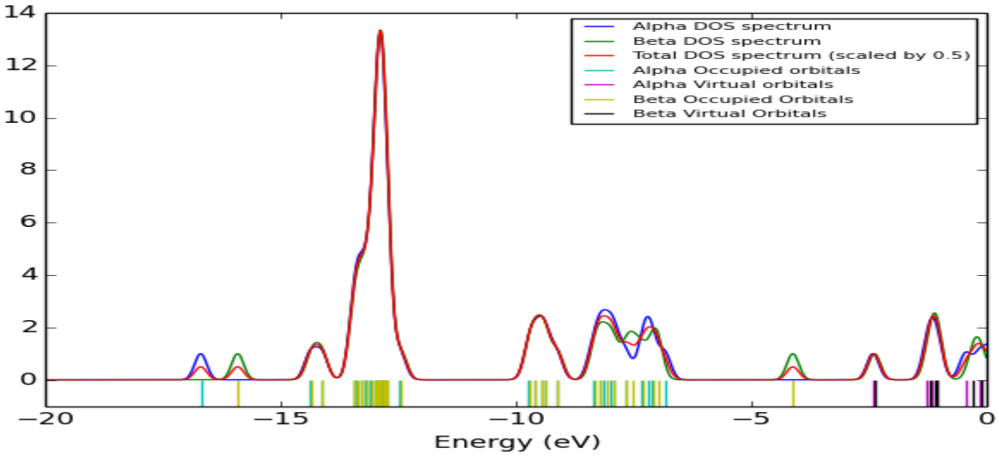


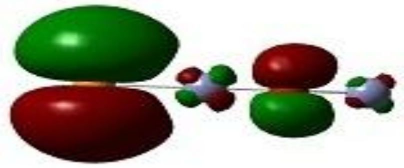
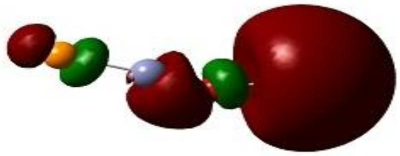
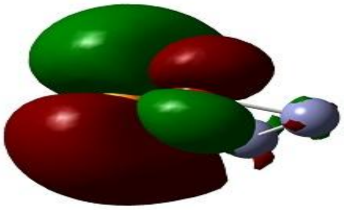
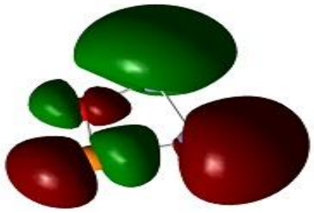
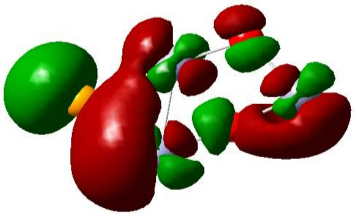
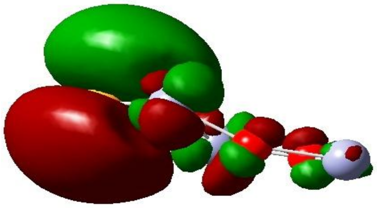
Figure 11(b): HOMO-LUMO, DOS spectrum of Zn_5O_4P micro cluster ring structure.

The DOS spectrum of Zn_5O_4P for linear, ring and 3D structures are shown in Fig. 11. It is shown that the accepter level is very low in the linear structure as compared to the other structures (ring and 3D). It indicates that for closed structures of Phosphorus doped ZnO, the accepter level is more than expected for the stable p-type conductivity. The HOMO-LUMO visualization is shown in table 7

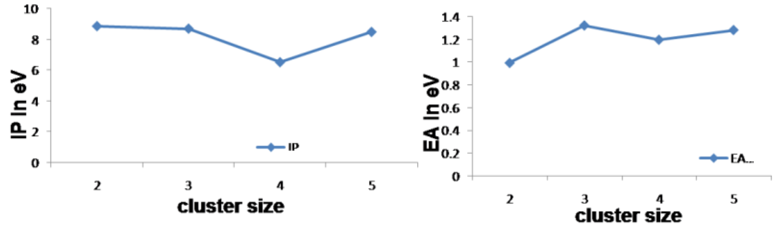
Table 6: HOMO-LUMO gap of $Zn_xO_{x-1}P$ (x=2-5).

Structure	Size	HOMO Alpha (eV)	LUMO Alpha (eV)	Gap (eV)	HOMO Beta (eV)	LUMO Beta (eV)	Gap (eV)
Linear	2	6.64	3.39	3.25	5.62	3.36	2.26
	3	6.63	3.42	3.21	5.64	3.38	2.26
	4	6.66	3.37	3.29	5.65	3.42	2.23
	5	6.60	3.34	3.26	5.61	3.43	2.19
Ring	2	6.22	3.28	2.94	6.02	3.65	2.37
	3	6.86	2.62	4.24	6.86	4.08	2.76
	4	6.79	2.41	4.39	6.89	4.12	2.77
	5	6.83	2.41	4.42	6.98	4.11	2.87
3D	3	5.35	3.12	2.23	5.27	3.63	1.64
	4	6.47	3.35	3.12	6.17	4.63	1.54
	5	6.39	3.41	2.99	6.33	3.57	2.76

Table 7:HOMO-LUMO visualization and spin states of $Zn_xO_{x-1}P$ micro clusters.

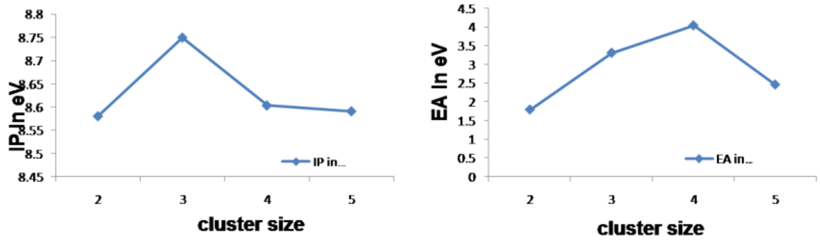
Cluster	Spin state	HOMO	LUMO
Zn_2O_1P Linear	Doublet		
Zn_2O_1P Ring	Doublet		
Zn_3O_2P 3D	Doublet		

The study of ionization potential (IP) and electron affinity (EA) are very important for micro clusters since they indicate the electronic structure of the cluster and also serves as a measuring tool for individual atomic to bulk behavior change. Ionization potential and electron affinity of different isomers provide important clues for identifying various low energy isomers. The IP and EA values for $Zn_xO_{x-1}P$ clusters are calculated from their orbital energies.



(a) Linear Structure

(b) Ring Structure



(c) 3D Structure

(c) 3D Structure

Figure 12: IP and EA of $Zn_xO_{x-1}P$ clusters-linear Structure **(b)** IP and EA of $Zn_xO_{x-1}P$ clusters-ring structure, and **(c)** IP and EA of $Zn_xO_{x-1}P$ clusters-3D structure.

Chapter 7: Conclusions

The work done in this thesis highlights following general conclusions:

A. Technological advantage and recent development in theory have enabled evolution of highly accurate, efficient and inexpensive methods that are applicable in the field of material science. In order to determine the stability of cluster, the use of the cohesive energy, energy change in a modal reaction, energy gap in electronic structure are studied. These parameters can be accurately computed with the help of DFT methods.

B. The variation of bond length and the number of atoms consisting of Ga_xAs_x (x=10,13,15,18,20,25,30) clusters was studied in detail. The other important parameters like binding energy; HOMO LUMO gap confirms the stability of the studied clusters. The optical activity is also discussed in detail.

C. Theoretical electronic structure techniques have become an indispensible and powerful means for predicting molecular properties and designing new materials. The density functional approach provides evidence for some specific fullerene-like cage molecules of semiconductor materials which exhibit high energetic stability and point group symmetry of Ga_xAs_x fullerene like clusters.

D. The principle of electrical properties is applied in the case of clusters by visiting some of the most influential studies. It is the main objective of the study to explore the stability of GaN clusters using the DFT.

E. The study of atomic structure and stability of $Cd_xS_{x\pm4}$ fullerenes like semiconductor cluster is done by using B3LYP method. It is found that the hollow fullerene like clusters are stable when the pentagon edges are shared to reduce the number of homo-nuclear bonds. The energetic and the energy gap in electronic structure are indicators for the stability of cluster. The study predicts that these clusters are stable. The stability of the cluster increases when the number of homo-nuclear bonds in the cluster is less.

The coefficients and different parameters used in different proposed theoretical model for semiconductor cluster can be easily computed by using computational quantum mechanical tools.

Experimental studies require a lot of resources like instruments, materials, environments etc. The computational techniques at molecular level through computational quantum mechanical tools help to propose specific type of molecule for designing and improving the electrical and optical properties of cluster.