ISSN (Online) 2393-8021
ISSN (Print) 2394-1588

International Advanced Research Journal in Science, Engineering and Technology
Vol. 2, Issue 11, November 2015

Structures Stabilities and Electronic Properties of GaAs Condensed Clusters

Deep Kumar[1], Rajkamal Shastri[2], Anil Kumar yadav[3], Devesh kumar[4]

Research Scholar, Dept of Applied Physics, School for Physical Sciences Babasaheb Bhimrao Ambedkar University, Lucknow, India[1, 2]

Assistant Professor, Dept of Applied Physics, School for Physical Sciences Babasaheb Bhimrao Ambedkar University, Lucknow, India[3]

Associate Professor, Dept of Applied Physics, School for Physical Sciences Babasaheb Bhimrao Ambedkar University, Lucknow, India[4]

Abstract: First-principal calculation are conceded out to appreciate the structural stability and electronic properties of nanotubes cluster and fundamental building blocks, Ga_nAs_n (n=1-3) small cluster by linear stacking of stable isomers, the condensed clusters, $(Ga_nAs_n)_m$ where n=1-3 and m =1-6 are modeled. The structure stability of condensed cluster their building blocks are achieved from the electron density of states. Electronic properties of all condensed cluster, with m≥4 are interesting in photo catalytic application as they have large energy gap than that of bulk. Our calculations also so that the $(Ga_3As_3)_m$ cluster are energetically more stable as compared with other condensed cluster.

Keyword: Carbon nanotubes, Density Functional Theory, Gallium arsenide.

I. INTRODUCTION

We are first going discussed carbon nano tubes (CNT) one dimension system gaining momentum with the invention of carbon nano tube (CNT). Appreciating that the potential application of CNT were due to their high mechanical strength ballistic transport and other novel properties (1) researches explored such as one dimensional system of inorganic compounds. For this above approach nanotubes and nanowires from Mo-S compound have been expansively studied and Even because of their many advantages for certain applications of CNTs has been suggested (2,3)as an alternative. Synthesis with unique structural and electronic properties and the ability to advance tune their properties by adding do pants (4). Recently, 1-D systems of CdS compounds have drawn much attention, leading to the synthesis of their nanowires,(5,6) nanotubes ,(7) and nanorods (8−10) with controlled dimensions.

As recently have proved that low dimensional semiconductor material have become a great interest to researcher in nanoscience among these material III-V group semiconductor compound have their paramount technological potential application such as photo electronic device, photonic integrations, ultrahigh frequency microwave and photovoltaic solar cells.

Gallium arsenide (GaAs) as substantial member of the III-V group semiconductor compounds has many distinctive properties as a low electronic effective mass high electron mobility and high saturation drift velocity which make it ideal for optoelectronic, low power and ultra high speed devices application more over it is an advantage material for making nanoscale devices because it surface Fermi level, pinning in the conduction band does not became an insulator due to depletion of carriers. Hence the post decades there have been a great number of studies investigating the chemical and physical properties of its nanostructure.

In the present work, we have investigated the atomic structure and electronic properties of condensed clusters and their infinite nanowires by first principles calculations within the construction of density functional theory.

II. COMPUTATIONAL

All GaAs and condensed clusters reported in this work are optimized by using the DFT with unrestricted B3LYP exchange-correlation potential. To superior describe the binding and geometrical feature of heavy atom, the basis set, effective core potential LanL2DZ, was adopted in this study for both arsenic (As) and gallium (Ga) atoms.. In this basis set the outermost electrons$3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^1$for Ga and $3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^1$ for As were described .the procedures of optimization were based on energy system convergence of energy was superior then10^{-6}(a.u. is atomic unit). In sequence to save time and improve efficiency the processes to optimize the structures with determined bond length ,bond angle, and dihedral angle of the initial value in the convergence criterion of 10^{-4}a.u. based on the optimized tube like clusters. All these calculation were implemented with the Gaussian 09 program package

The binding energy per atom (BE) of cluster is calculated from

$$\text{BE}=\frac{nE(Ga)+nE(As)-E(Ga_nAs_n)}{2n}$$

Where E(Ga), E(As)and $E(Ga_nAs_n)$ are the total energy of a single Ga atom, a single As atom and Ga_nAs_n clusters respectively and nis the number of Ga or As atoms.

ISSN (Online) 2393-8021
ISSN (Print) 2394-1588
International Advanced Research Journal in Science, Engineering and Technology
Vol. 2, Issue 11, November 2015

Similarly calucalation are extended to condensed cluster we also agreed out the firest principal calculation on infinite Ga_nAs_n nanowires with n=1-3 for the sake of comparision

III. RESULTS AND DISCUSSION

We conceded out first principal calculations on various Ga_nAs_n (n=1-4) cluster, to obtained the stable isomers in each size range, which act as building blocks of condensed cluster . The optimized structure are shown in fig. and the BE, HOMO-LUMO gap, Cd−S bond distance, and bond angle of stable isomers are reported in Table 1

Condensed Clusters With a information of stable isomers of Ga_nAs_n in each size range, condensed clusters of $(Ga_nAs_n)_m$ are achieved by linear stacking of m (up to 6) units of stable Ga_nAs_n isomers (n = 1−3). We also effort the condensed of the stable isomer of Ga_5As_5 but the significant structural distortion observed due to a larger cavity in the center of the ring. Hence we did not progress further.

The optimized structures of condensed clusters are shown in fig 1. the $(Ga_3As_3)_2$ clusters is obtained by condensing a planer Ga_3As_3 cluster at the top and another cluster at the bottom, thus increasing the number Ga-As bonds in the cluster. In a similar way $(Ga_3As_3)_4$ and other condensed cluster, $(Ga_nAs_n)_m$ are obtained and optimized structures are shown in figure.

We calculate the BE and HOMO-LUMO gap of all condensed $(Ga_nAs_n)_m$ cluster, and the results are shown in table1. Along with the cohesive energy per atom and band gap of infinite Ga_nAs_n nanowires. As estimated the BE of condensed cluster increases with m and slowly reaches the cohesive energy of the corresponding infinite nanowires, as seen in table 1. Nanorods and infinite nanowires.

In the inset the Bes of condensed cluster with respect to the diameter (in terms of n) are shown. Hence it conclusion that the $(Ga_3As_3)_m$ condensed clusters are more stable as compared to other-sized condensed clusters and this cluster could preferably extend to the HOMO−LUMO gap decreases, beyond m = 2.

Table 1 showing HOMO-LUMO gap, Bond length (Ga-As) and binding energy of the cluster. **(a)** $(GaAs)_m$ cluster, **(b)** $(Ga_2As_2)_m$ cluster, **(c)** $(Ga_3As_3)_m$ cluster

(a)

Structure	Energy Gap eV	Bond length (Ga-As) A^0	Binding energy (eV)
(GaAs)2	1.89	2.39-2.51	2.10
(GaAs)3	0.56	2.49-2.52	2.01
(GaAs)4	0.53	2.38-2.52	2.36
(GaAs)5	0.40	2.36-2.39	2.40
(GaAs)6	0.53	2.38-2.51	2.43

(b)

Structure	Energy Gap eV	Bond length (Ga-As)	Binding energy (eV)
$(Ga_2As_2)_2$	2.05	2.54-2.71	2.60
$(Ga_2As_2)_3$	2.30	2.41-2.55	2.78
$(Ga_2As_2)_4$	1.39	2.53-2.58	2.82
$(Ga_2As_2)_5$	1.09	2.52-2.59	2.87
$(Ga_2As_2)_6$	0.57	2.53-2.62	2.56

(c)

Structure	Energy Gap eV	Bond length (Ga-As)	Binding energy (eV)
$(Ga_3As_3)_2$	1.48	2.53-2.58	2.85
$(Ga_3As_3)_3$	1.46	2.53-2.62	2.86
$(Ga_3As_3)_4$	1.11	2.53-2.56	2.88
$(Ga_3As_3)_5$	1.94	2.48-2.54	3.00
$(Ga_3As_3)_6$	1.12	2.57-2.59	2.90

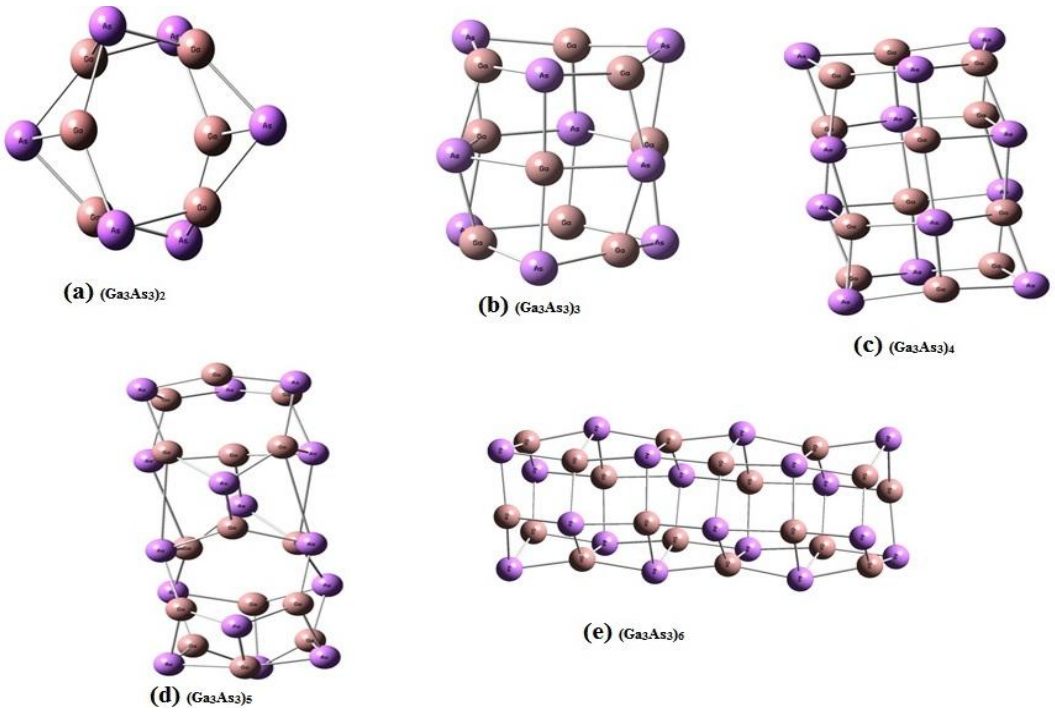

Fig.1 The optimized structure of $(Ga_3As_3)_m$ condensed clusters. (a) $(Ga_3As_3)_2$ (b) $(Ga_3As_3)_m$ (c) $(Ga_3As_3)_m$ (d) $(Ga_3As_3)_m$ (e) $(Ga_3As_3)_m$ are shown.

DOI 10.17148/IARJSET.2015.21121

ISSN (Online) 2393-8021
ISSN (Print) 2394-1588
International Advanced Research Journal in Science, Engineering and Technology
Vol. 2, Issue 11, November 2015

Figure 2 shows the variation of the HUMO−LUMO gaps of the condensed clusters. For the $(Ga1As1)_m$ atomic wire, We find that the decrease in the gap is mainly due to variation in the LUMO of atomic wires, which is quite similar to a linear polyene system. Similarly, for n = 2, 3, and 4, the HOMO−LUMO gap decreases as the m value increases. It is interesting to observe that, beyond m = 4, the HOMO−LUMO gap for $(Ga_3As_3)_m$ condensed clusters is significantly higher than that of other condensed clusters (including infinite nanowires). This supports our earlier statement that $(Ga_3As_3)_m$ condensed clusters are the most stable among all other clusters. Further, we also noted in Figure 2 that, beyond m = 5, the HOMO− LUMO gap of the $(Ga1As1)_m$ atomic wire is less than that of other condensed clusters. It is a consequence of the increase in the number of nonbonding states with the increase in the length of the atomic wire. Overall, the HOMO−LUMO gap of all $(Ga_nAs_n)_m$ condensed clusters, beyond m = 4, is less than the band gap of the bulk GaAs compound. Hence, the photo catalytic activity of these clusters is expected to be higher when compared with that of the bulk.

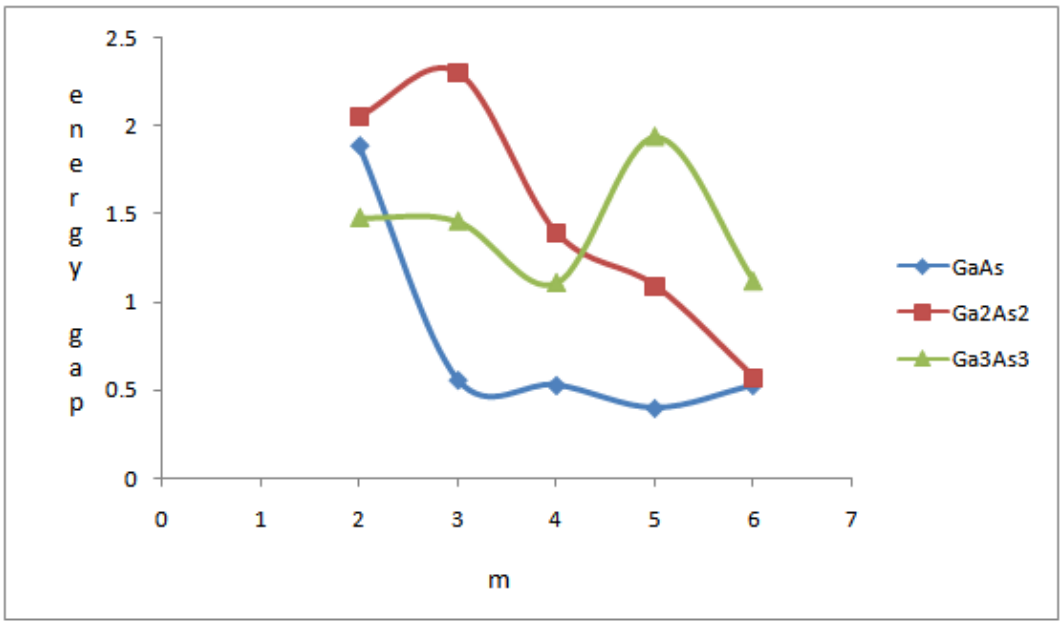

Fig.2. showing HOMO-LUMO gap of $(Ga_nAs_n)_m$ are shown.

IV. CONCLUSION

We studies the structure stablity and electronic properties of $(Ga_nAs_n)_m$ (n=1-3,m=1-6) condensed cluster and their building block from firest-principal calculation . the structual stablity of cluster is explain by the HOMO – LUMO gap and Bes. Further, electronic properties of condensed clusters with m > 4 show a lower energy gap as compared with the bulk GaAs system, and it would be interesting in photo catalytic applications. Our calculations also reveal that the condensed clusters have more structural stability as compared to 1-D nanorods obtained from the bulk in this dimension.

REFERENCES

1. G Dresselhaus, M S Dresselhaus, P Eklund, Science of Fullerenes and Carbon Nanotubes; Academic Press: San Diego, CA, 1995.
2. Y Feldman , E Wasserman, D J Srolovitz, R Tenne High-Rate, Gas-Phase Growth of MoS2 Nested Inorganic Fullerenes and Nanotubes. R. Science 1995, 267, 222−225
3. V. Nicolosi, P. D Nellist, S. Sanvito, E. C. Cosgriff, S. Krishnamurthy, W. J. Blau, M. L. H. Green, D. Vengust, D. Dvorsek, D. Mihailovic, G. Compagnini, J. Sloan, V. Stolojan, J. D Carey, S. J Pennycook And J. N. Coleman, Aberration Corrected Electron Microscopy Reveals van der Waals Driven Self-Assembly Of MoSI Nanowires into A Low Symmetry Structure", in Advanced Materials, 2007, 19, 543 – 547.
4. P Murugan, V Kumar, Y Kawazoe, N Ota Ab initio study of structural stability of Mo-S clusters and size specific stoichiometries of magic clusters, Physical Chemistry A 111 (14), 2778-2782.
5. JH Zhan, XG Yang, WX Zhang, DW Wang, Y Xie, YT Qian, A solvothermal route to wurtzite ZnSe nanoparticles Journal of Materials Research 2015 (03), 629-632.
6. Jinyou Xu, Xiujuan Zhuang, Pengfei Guo, Qinglin Zhang, Weiqing Huang, Qiang Wan, Wei Hu,Xiaoxia Wang, Xiaoli Zhu, Changzeng Fan, Zongyin Yang, Limin Tong, Xiangfeng Duan, and Anlian Pan, Wavelength-Converted/Selective Waveguiding Based on Composition-Graded Semiconductor Nanowires Nano Lett. 2012, 12, 5003−5007.
7. Hui Zhang, Deren Yang, Yujie Ji, Xiangyang Ma, Jin Xu, and Duanlin Que Low Temperature Synthesis of Flowerlike ZnO Nanostructures by Cetyltrimethylammonium Bromide-Assisted Hydrothermal Process ACS Nano 2010, 4, 91−98
8. Zhang, H.; Ma, X. Y.; Xu, J.; Yang, D. R Synthesis and Characterization of CdS, ZnS and CdZnS Nanoparticles Embedded in Polystyrene, j. Cryst. Growth 2004, 263, 372−376.
9. A.E Saunders,A Ghezelbash, P Sood, B Korgel, Synthesis of high aspect ratio quantum-size CdS nanorods and their surface-dependent photoluminescence. A. Langmuir2008, 24, 9043−9049.
10. A S Barnard, Xu, H. Modelling polar wurtzite ZnS nanoparticles: the effect of sulphur supersaturation on size- and shape-dependent phase transformations J. Phys. Chem. C 2007, 111, 18112− 18117