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# STUDY OF ELECTROSTATIC POTENTIAL SURFACE AROUND BIPYRAMIDAL GaAs QUANTUM DOT

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Semiconductor quantum dot have got scientific interest because of their unique electronic nature. In this article, an isolated square bipyramidal gallium arsenide (GaAs) quantum dot has been optimized using DFT method. The size of quantum dot was 1.2 $nm^2$ (square base) and 1.7nm height and consisted of total 84 atoms. The quantum dot was optimized using hybrid B3LYP functional and SBKJC pseudo potential basis sets. The electrostatic potential surface around the optimized GaAs quantum dot was plotted and the result showed the potential on the pyramid surface was polarized with two positive and negative surfaces. This potential was due electronic and nuclear charge of different arrangement on the surface structure of the dot.

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## 1. Introduction

Electrostatic potential is associated with a charge distribution and can be defined as the potential energy of a test particle per unit charge of the particle. At molecular level, the electrostatic potential has been studied to determine the interaction of the molecule with its surrounding. The electrostatic potential study also explains the electronic distribution and structure formation of a molecule. Various studies about molecular electrostatic potential have been carried out to enlighten the behavior and interaction of the molecules to its environment. In chemical and biological field this phenomenon has been employed to studying the interaction of molecule such as protein, DNA and vaccine [1-5]. In physics it is mainly focused towards the electronic part such as the interaction of potential energy surface with charge particle and the development of nanodevices. *Lis et.al* have studied gated quantum dot to tune the confinement potential for nanodevices [6]. Whereas, the others groups measured the potential distribution around probe tip as instrument development [7-8].

The focus of the present study is to explore the role of electrostatic potential in Single Electron Transistor (SET), which is vital in SET development. The main phenomenon behind the working of SET is tunneling of electron. Many studies have been conducted to simulate the tunneling phenomena [9-12] and *Boese et.al* has concluded in their study that the electron tunneling through molecular nano-devices is inevitably controlled by its electronic and mechanical structure [13]. Due to quantum mechanical behaviour of tunneling, the interaction of the single electron tunneling to the quantum dot is still unclear. In this paper, the electrostatic potential surface around isolated GaAs bipyrimidal quantum dot is presented. This study will give an insight on behavior of the single electron interaction with the quantum dot during the tunneling to the quantum dot process.

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## 2. Method and theory

GaAs quantum dot was optimized using GAMESS-US [14] software which works within the frame work of density functional theory (DFT). The GaAs quantum dot was consisted of total 84 atoms and arranged in zincblende structure as shown in figure 1. The optimization process was done with B3LYP (Becke, three-parameter, Lee-Yang-Parr) functional and SBKJC (Stevens/Basch/Krauss/Jasien/Cundari) pseudo potential basis sets [15]. DFT method with B3LYP functional approximations which is one of the most accurate schemes widely used to calculate the molecular geometry optimization [16-18]. The pseudo potential basis sets was used in the optimization because the computation of full orbital calculation would be very expensive. The electrostatic potential was calculated using the optimized structure.
The electrostatic potential at position **r** is given as a sum of contributions from the nuclei and the electronic wave function;

$$V(r) = \sum_{nuclei}^{A} \frac{Z_A}{| r - R_A |} - \int \frac{| \psi(r_i) |^2}{| r - r_i |}$$

where, $Z_A$ is the charge of nuclear, $\mathbf{R}_A$ is nuclear position, $\mathbf{r}_i$ is electronic position and ψ is the molecular electronic wave function. The first part of the potential was trivially calculated from the nuclear charges and their position and the electronic contribution was from the molecular wave function. The electrostatic potential was calculated at grid point around the quantum dot and the equipotential surface is plotted. The electrostatic potential surface is plotted in 3D using MacMolPlt package which was developed by Brett Bode [19].

## 3. Results and discussion

GaAs quantum dot which comprises 84 atoms has been optimized using DFT method. The simulated quantum dot was in an isolated system (without substrate) and had the square bipyramidal shape. The square base of the bipyramidal had an area of 1.44 $nm^2$ and length between the two tip of the pyramid was 1.7nm. The atomic arrangement in the optimized dot was exactly the same as the bulk GaAs which was zincblende structure.

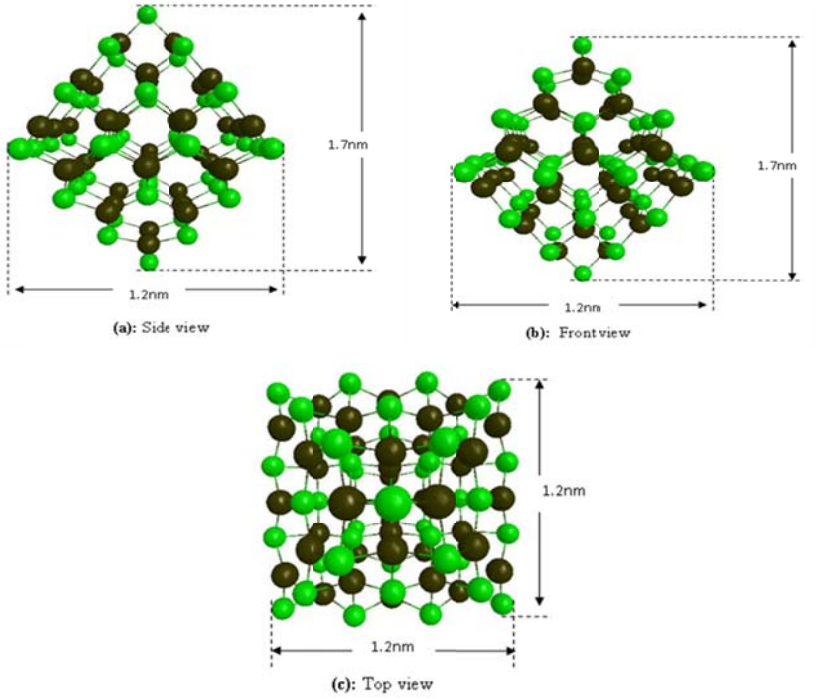


*Fig 1: (a) Side view (b) front view and (c) top view of optimized GaAs quantum dot structure.*

The optimized GaAs quantum dot is presented in figure 2. The potential around the quantum dot is drawn 3D using MacMolPlot program with three different angles related with figure 1 (side, front and top). There is four different value of potential contour for each set of angles from 1.0 Hartree to 0.001 Hartree. This contour (the red/blue surface) is the isosurface of the potential value and all the point at the contour surface has the same value of electrostatic potential. The color represents the sign of potential i.e. red is the positive potential surface and blue is the negative potential surface.

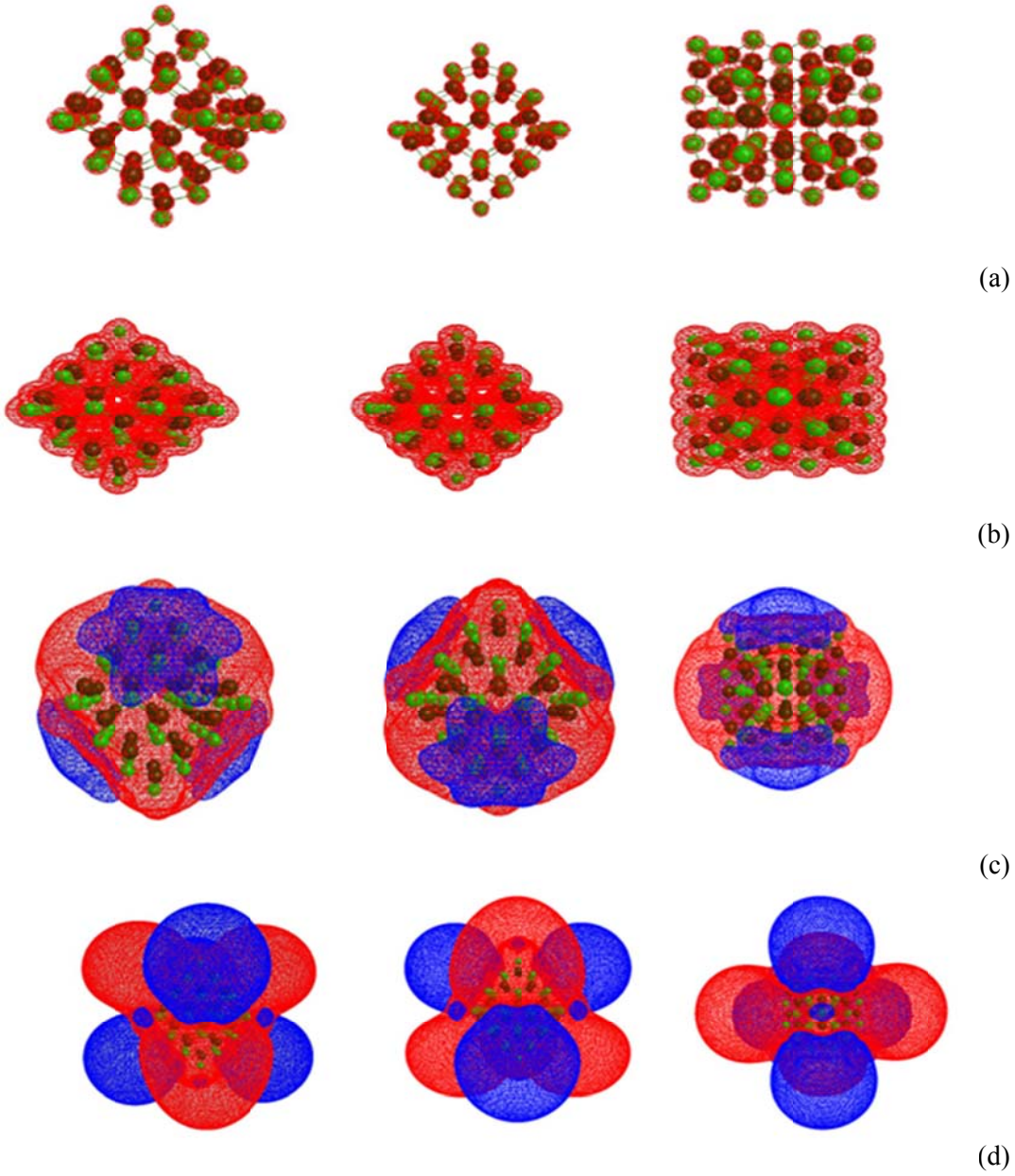


*Fig 2: (a) (b) (c) (d) 3D electrostatic potential surface of optimized GaAs quantum dot structure.*

Figure 2 shows that electrostatic potential with high positive value just around each atomic coordinate as shown by figure 2 (a). As the potential value decreases the isosurface moves away from the atomic coordinate and saturates around the dot (Figure 2-b). The electrostatic potential at 0.010 Hartree, the blue surface is seen which indicates the negative potential surface which is wrapping around the dot. The same goes to potential of 0.001 Hartree and the surface becoming larger and expanding.

In figure 2 (a) and (b), the electrostatic contour value is large which means the potential surface should be just around the nucleus of Ga and As atoms. The contribution of the positive potential was mainly by the positive charge in the nucleus. As the value of electrostatic potential decreases, the isosurface expands further from the atomic coordinates and the negative value of electrostatic potential is emerged (blue) such as in figure 2 (c) and (d). This electrostatic potential surface now influences by the electronic part of the dot.

The electrostatic potential surface (figure 2 (c) and (d)) is mainly due to the electronegativity and partial charges of the element in the dot. Since the As element is closer to Fluorine in the periodic table, therefore, As atoms are more electronegative than Ga. At the same time electronegativity of atoms in molecules indicates likelihood of the partial charges to be found. The most electronegative atoms are most negative, the other are less or more positive.

In this particular quantum dot, there were two type surface structures and lets concentrates on the top square pyramid of the dot. First one consists of As atoms only as shown in the left and right faces of the top pyramid from the front view (figure 1 (b)). The second surface consists of both Ga and As atoms at the left and right face of the top pyramid from the side view (figure 1(a)). Thus it is clear that the surface with the As atoms is more electronegative than the other one. The more positive side has Ga on the surface thus more nuclei on the surface which contribute to the more positive potential. This positive region also indicates that the nuclear charge in this area is incompletely shielded by the electrons.

## 4. Conclusions

An isolated bipyramid GaAs quantum dot has been optimized. Its structure is zincblende just like the bulk GaAs material's structure. The dot has two different surface structures from the eight surface of the bipyramid. This arrangement gives the different (positive and negative) potential surface around the dot. The potential is due to the distribution of the Ga and As atoms on the surfaces of the quantum dot. The electronegativity of As atoms contribute to negative potential surface and the positive potential around the dot is contributed from the lack of electron shielding on the surface. The results give an insight on how the electrons will travel towards the square pyramidal shape quantum dot and this result will give good geometrical information for SET development.

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