

An Analysis of the Electron Trajectory in the Vicinity of GaAs Quantum Dot (Analisis Lintasan Pergerakan Elektron di Sekitar Titik Kuantum GaAs)

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ABSTRACT

Quantum dots being an interesting class of nanostructures are considered potential prototype systems for novel nano-devices such as single electron transistor (SET). Here in this research, we present an analysis of the electron trajectory in the vicinity of gallium arsenide (GaAs) quantum dot. To perform this study, DFT based methodology is employed to optimize structure of quantum dot and determining the electrostatic potential around the dot. Under the influence of obtained electrostatic potential, trajectory of the moving electron towards the dot is investigated. The results showed that GaAs quantum dot have negative and positive potential surfaces that influence the electron interaction with the dot. These results motivate the development of SET electrode channel where the electron moves towards the dot on the surface with positive potential rather than negative potential surface.

Keywords: Density functional theory; electron trajectory; GaAs; quantum dot

ABSTRAK

Titik kuantum adalah kelas struktur nano yang menarik dan dianggap berpotensi sebagai sistem prototip untuk peranti-nano seperti transistor elektron tunggal (SET). Dalam kajian ini kami melaporkan analisis lintasan elektron di sekitar titik kuantum galium arsenida (GaAs). Dalam kajian ini, kaedah DFT digunakan untuk mengoptimumkan struktur titik kuantum dan mengira keupayaan elektrostatik di sekeliling titik kuantum. Di bawah aruhan keupayaan elektrostatik yang didapati, lintasan pergerakan satu elektron menuju ke titik kuantum dikaji. Hasil kajian menunjukkan bahawa titik kuantum GaAs mempunyai permukaan keupayaan positif dan negatif yang mengaruh interaksi antara elektron dan titik kuantum. Hasil kajian ini memotivasikan pembangunan saluran elektrod SET dengan elektron bergerak menuju ke arah titik kuantum pada permukaan keupayaan positif berbanding permukaan berkeupayaan negatif.

Kata kunci: GaAs; lintasan elektron; teori fungsi ketumpatan; titik kuantum

INTRODUCTION

In the recent years, many materials research are devoted, both experimentally and theoretically, to nano-particles (for instance, quantum dots, nanorods and nanofilms) (Drbohlavova et al. 2009) because of their promising industrial and scientific applications for example in textiles, coatings, biotechnology, health care, catalysis, data storage, biomedical, pharmaceutical and quantum computing. Quantum dots, one of the important class nano-particles, categorized as zero dimension (0D) nanostructures, are being extensively investigated. The peculiarity of quantum dots (QDs) is that their electronic and optical properties can be tailored for different purposes using the same material by simply changing the size of dot that have made them more celebrated in the area of nanotechnology. Due to the size dependence properties of QD, this nanostructure is also known as an artificial atom. Though quantum dots mostly are used in biological systems, recently novel applications of CdS-QDs and CdTeS-QDs in solar cells made it more promising for optoelectronics applications as well. Moreover QDs are also predicted as prototype systems for novel nano-devices for example, single electron transistor (SET) (Kastner 2000), semiconductor

laser diode (LDs) (Huffaker et al. 1998; Kirstaedter et al. 1994), semiconductor optical amplifiers (SOA) (Akiyama et al. 2003; Sugawara et al. 2004) and photodetector (Liu 2003).

In literature, though some studies have been reported about metallic and metalloid QDs (Fujioka et al. 2008), most of the investigations deal with semiconductor materials. From several types of semiconductor QDs, GaAs is one of the most widely studied systems. It is due to its inherent superior electronic properties like higher carrier mobilities/saturated electron velocity besides small effective mass, stability and flexibility for multiple heterojunctions that are crucial in constructing fast microelectronic devices (Howes & Morgan 1985). Experimentally GaAs-QD have been fabricated and investigated using various techniques (Arashida et al. 2010; Kuroda et al. 2010; Lee et al. 2006), whereas previously reported theoretical research is mostly dedicated to GaAs clustering (Gosh et al. 2005; Karatzer et al. 1998; Sun et al. 2003) and addresses characterization and properties of GaAs-QD.

SET as the name suggest, is fast switching devices which operate using single electron in transistor operation. The main theory behind the SET device is quantum

mechanical electron tunneling phenomenon. Though some studies have also been done to model and simulate the single electron tunneling process (Blick et al. 1996; Boese & Schoeller 2001; Glazman 2000; Gupta & Saraf 2009; Schouteden et al. 2008), the trajectory of the single electron tunneling within the quantum dot is still unclear. Knowledge of electrostatic potential of QDs plays fundamental role in device simulation such as SET and in determining the trajectory of the single electron tunneling. Therefore a study about the calculations of electrostatic potential of QD is necessiated.

In our previous work, investigations about the electrostatic potential surface around GaAs-QD without an external electric field were presented (Hanafi et al. 2012). We extend our briefly reported study in this paper, to the calculations of electrostatic potential and the electron trajectory due to electrostatic potential around isolated GaAs bipyramidal QD. The emphasis of this paper was therefore to explore the role of electrostatic potential in guiding the electron trajectory that moves towards an island in single electron transistor (SET). This study will give more information on the mechanism of single electron interaction with the quantum dot during the tunneling process.

METHODS

The main demand in the usage of nanosized devices is to produce devices with low power consumption and of better performance. Although it has recently been possible to produce the quantum dot nanodevices, experimental study of the properties of these devices due to small size is still expensive. This study is performed therefore via simulation using state of the art first principles quantum mechanical cost effective methods.

Frist principles DFT simulation tools are broadly use in device fabrication as well as the characterization of materials at all length scales from bulk to QDs, however quality of the DFT mainly rely on the suitable choice of exchange correlation functional approximation. DFT

based methodologies at the level of B3LYP functional approximation is considered one of the most accurate schemes and is widely used to calculate the molecular geometry optimization (Burrill & Grein 2005; Karamanis et al. 2007; Li & Huang 2003). In this recent work we have applied hybrid density functional theory (DFT) at the level of B3LYP (Becke, three-parameter, Lee-Yang-Parr) as an exchange-correlation functional and SBKJC (Stevens/Basch/Krauss/Jasien/Cundari) pseudo potential basis sets (Stevens et al. 1992) as implemented in a software package GAMESS-US (Schmidt et al. 1993). The optimized structure of GaAs-QD consists of total 84 atoms and are arranged in zinc blend (ZB) structure as shown in Figure 1.

In this structure Ga and As atoms are lying on alternative inter-penetrating face centered cubic (fcc) lattices. The total number of electrons contributed by Ga, 31 and As, 33 are 2692 in this QD. The electrostatic potential at position r as a sum of contributions from the nuclei and the electronic wave functions is given;

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

where, Z_A is the charge of nuclear, R_A is nuclear position, 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 positions whereas electronic contribution was found out from the molecular wave function. The electrostatic potential was calculated at grid point around the QD and corresponding equipotential surface is plotted. By the application of MacMolPlt package, 3D electrostatic potential surface is plotted, developed by Brett Bode (Bode & Gordon 1998).

The calculated potential of the GaAs-QD by the application of above mentioned DFT approach as implemented in GAMESS code is synchronized with the Source-Drain-Gate potential obtained from Java program which is developed to mimicking the SET electrode. To do so, the starting point is selected around the source electrode and the potential at

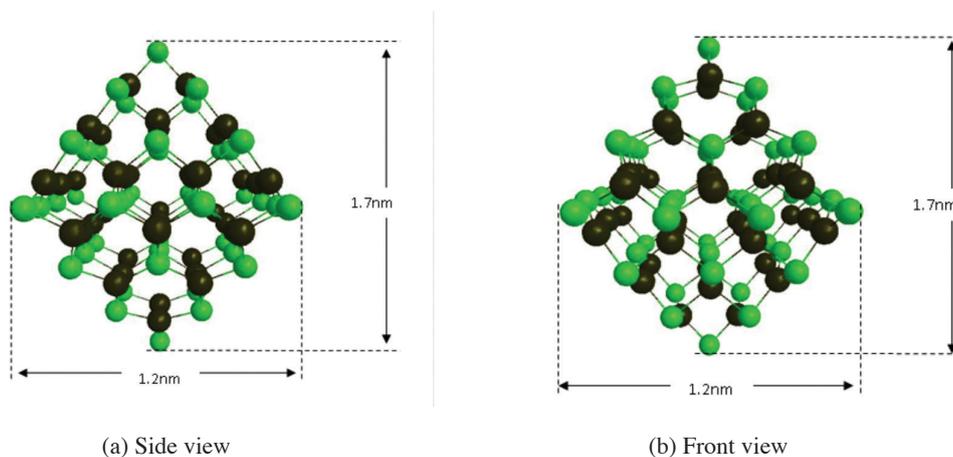


FIGURE 1. Optimized ZB-GaAs bipyramidal QD: (a) side view and (b) front view

that point is recorded as V_{max} . From the starting points, the program will scan through all 26 neighbor point around the starting point for the highest potential. Thus the next point for the electron to go is the highest potential point. Assuming there are higher points after the starting point, the program will go into loop which scans including the next point and changing the potential, V_{max} . If there is no highest potential obviously the starting point is at the highest potential thus the electron is not going anywhere.

At the position far from the dot, electron is expected to move towards the dot because the potential is lower at the source electrode and higher at the drain electrode. When the electron approaches towards the dot, it is expected that there will be some changes or alteration in potential due to potential affected by the dot. Thus the developed JAVA program is also taking account for the fluctuations of the next point. If the electron has reached the highest potential point, then the program will extrapolate the path of the electron to the next point and next two points in the path. This is assumed to be going on as long as the electron has enough energy (the velocity $v \neq 0$) to move in that direction. The program will stop if the electron arrives to the limit such as the 3D potential box barrier or the electron is moving in the same circle of path over and over again. The recorded point of the electron path is then

analyzed and plotted using GNUPLOT program and the result is discussed.

RESULTS AND DISCUSSION

From the optimized GaAs quantum dot shown in Figure 1 the electrostatic potential around the quantum dot is plotted in Figures 2 and 3. The 3D potential plot is made using MacMolPlot program and plotted from three different angles as can be seen from Figures 2 and 3. This contour (the red/blue surface) is the iso-surface of the potential value which means that all points on the contour surface have the same value of electrostatic potential. The red color represents positive potential surface and blue is for the negative potential surface. This electrostatic potential is due to accumulative effects of electronegativity and partial charges of the elements present in the QD. Using the information obtained from this electrostatic potential surface, the trajectory of an electron is analyzed using a computer program as developed in Java language. The path followed by the external electron while moving around the dot is plotted using Gnu-plot as shown in Figures 4-6. Figure 4 shows the plotted surface with the contour of the isosurface using the 2D potential plot. The contour shape is the same as the plotted electrostatic potential surface

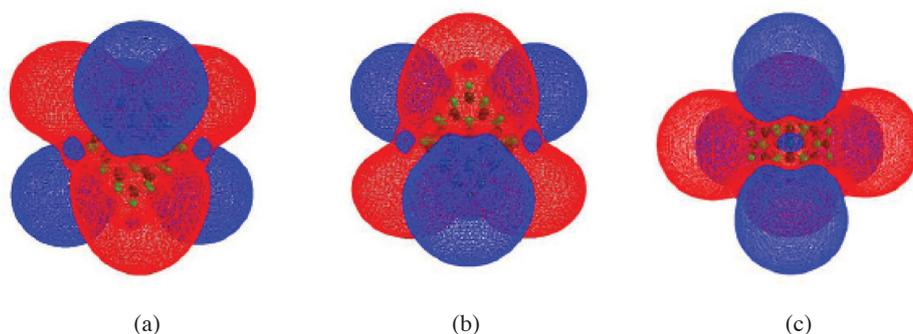


FIGURE 2. Electrostatic potential surface plot from GaAs without external electric field

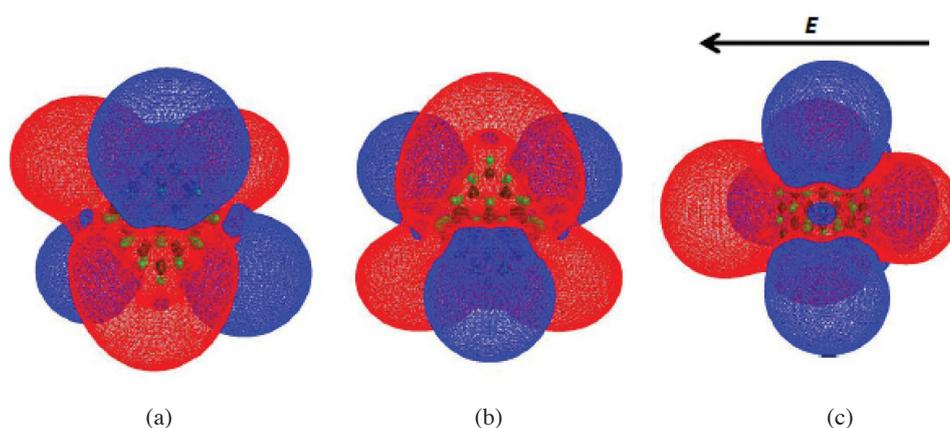


FIGURE 3. Electrostatic potential surface plot from GaAs with external electric field

in Figures 2-3. As our main research interest is in the electron movement path, therefore Figure 4 is zoomed to the selected area and the result is shown in Figure 5.

Figure 5 shows the main area that influences the movement of the electron. The electron ejected from the electrode is pulled towards the center of the dot as the potential surface, in front of the dot, is of spherical shape. Thus the electron movement toward the higher potential surface is always tangential to the plotted isosurface. This can easily be seen by viewing same plot from another angle as shown in Figure 6. The top view shows that the electron movement is tangential towards the center of the dot and then move along a straight line towards the dot.

As the electron steps forward, its movement is itself affected by the shape of the dot. As the dot is an inclined plane as seen by the ejected electron, so, at lower level of the dot, more atoms are around it and therefore more electrons compared with the top of the dot. Thus, the electron goes higher up until the point where the nucleus was exposed due to lack of electron shield. At this point the ejected electron is suck towards the nucleus of the Ga which was explained earlier for the atoms with fewer electrons shielding (Figure 6).

Figures 6 and 7 show the end of the electron movement which has been in loop around (in 3D) the very high potential. This high potential is due to the nucleus of the

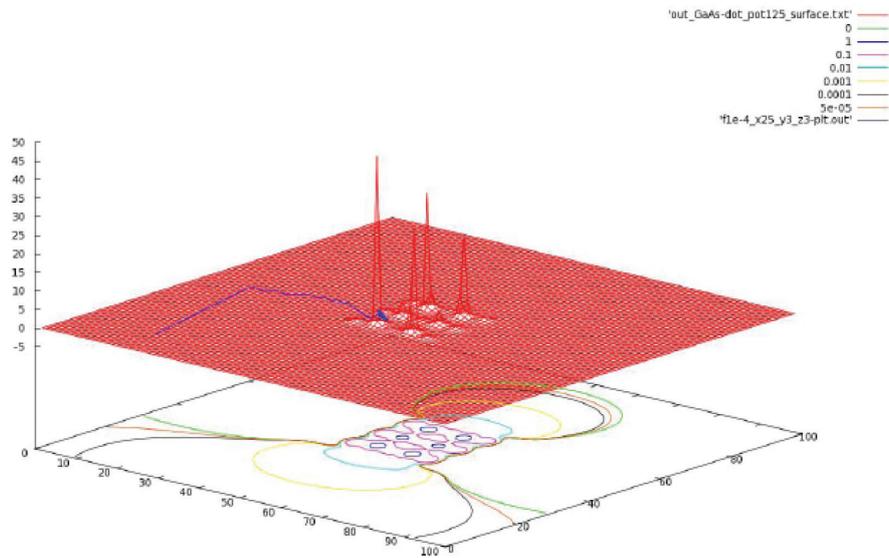


FIGURE 4. Electron movement path (blue line) and a layer of 2D electrostatic potential plot with contour

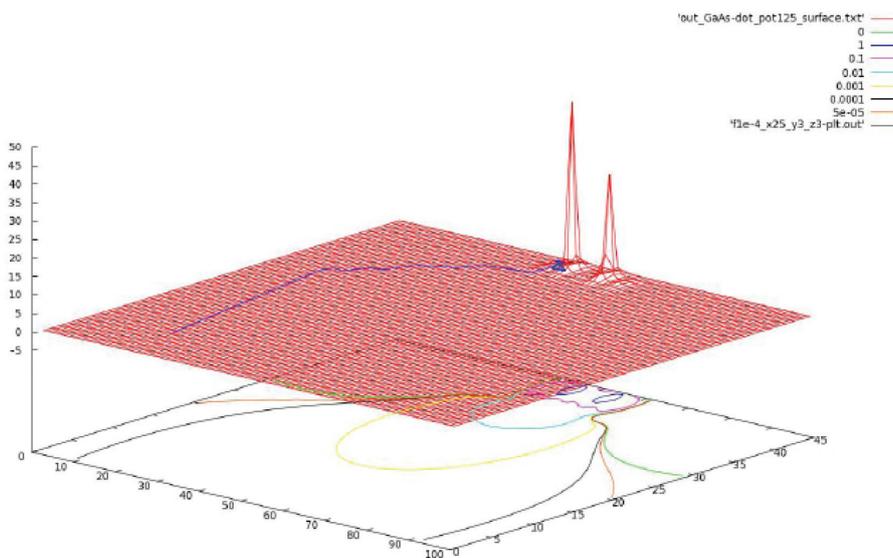


FIGURE 5. Zoom in for electron movement path (blue line) and a layer of 2D electrostatic potential plot with contour

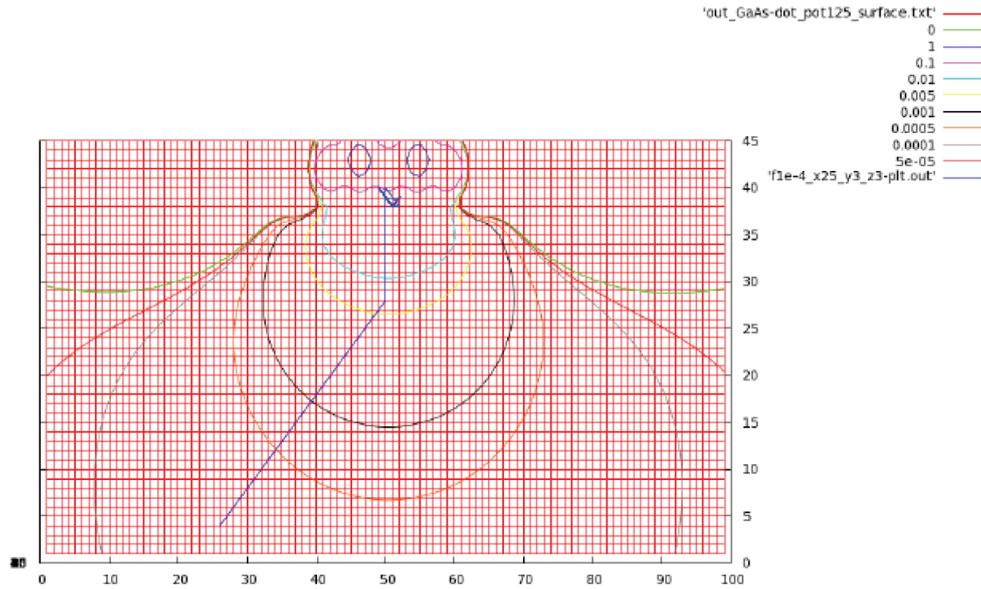


FIGURE 6. Zoom in for electron movement path (blue line) from the top view and a layer of 2D electrostatic potential plot with contour

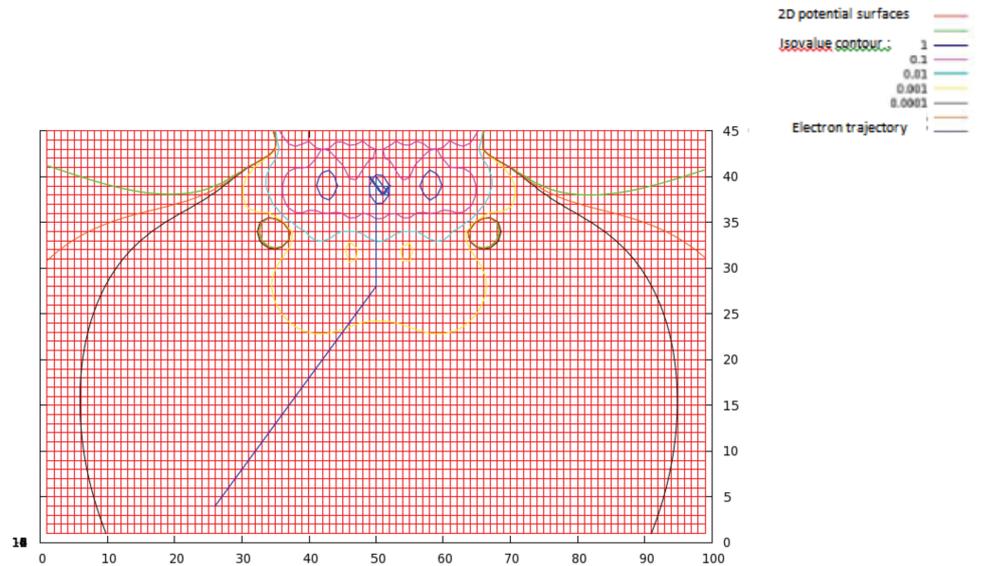


FIGURE 7. Zoom in for electron movement path (blue line) from the top view and a layer of 2D electrostatic potential plot at the same level with the end of electron trajectory

Ga atom at that point. From the SET point of view this might be not good as the electron cannot pass through from source to drain electrode. This might be due to the application of various assumptions such as temperature, dynamic interaction and other limitations that have been imposed to study the system.

CONCLUSION

In conclusion, DFT based methods at the level of B3LYP exchange correlation functional approximation was applied to optimize the GaAs-QD and to find out the electrostatic

potential of optimized dot. The movement of electron around the dot is determined under the influence of electrostatic potential around the dot. Our results showed that at first the electron moves towards the center of the plotted space and then inwards towards the dot. This means that the direction of electron movement is always tangential to the isosurface potential. At the end, the electron stuck on the middle of the surface of QD. This may be due to the very high positive potential produced by one of the Ga atom in the path of the electron movement. This might be happened due to the limitations and assumptions introduced in this study. Therefore to improve this result

future study demands to include the effect of dynamic of molecular vibration.

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REFERENCES

- Akiyama, T., Kawaguchi, K., Sugawara, M., Sudo, H., Ekawa, M., Ebe, H., Kuramata, A., Utsubo, K., Morito, K. & Arakawa, Y. 2003. *29th Euro.conf.on Opt.Comm. (ECOC)*, Rimini Fiera, postdeadline paper.
- Arashida, Y., Ogawa, Y. & Minani, F. 2010. Correlated photon from multi-carrier complexes in GaAs quantum dot. *Superlattices and Microstructure* 47: 93-97.
- Blick, R.H., Haug, R.J., Weis, J., Pfannkuche, D., Klitzing, K.V. & Eberl, K. 1996. Single electron tunneling through a double quantum dot: The artificial molecule. *Phys. Rev. B: Condensed Matter* 53(12): 7899-7902.
- Bode, B.M. & Gordon, M.S. 1998. Macmolplt: A graphical user interface for GAMESS. *J. Mol. Graphics Mod.* 16(12): 133-138.
- Boese, D. & Schoeller, H. 2001. Influence of nanomechanical properties on single-electron tunneling: A vibrating single-electron transistor. *Euro. Phys. Lett.* 54(5): 668.
- Burrill, S. & Grein, F. 2005. Structure and Bonding of III/V compounds X₂Y₂, with X=B, Al, Ga, and Y=N, P, As. *Journal of Molecular Structure (Theochem)* 757(1-3): 137-142.
- Drbohlovova, J., Adam, V., Kizek, R. & Hubalek, J. 2009. Quantum dots - characterization, preparation and usage in biological systems. *Int. J. Mol. Sci.* 10(2): 656-673.
- Fujioka, K., Hiruoka, M., Sato, K., Manabe, N., Miyasaka, R., Hanada, S., Hoshino, A., Tilley, R.D., Manome, Y., Hirakuri, K. & Yamamoto, K. 2008. Luminescent passive-oxidized silicon quantum dots as biological staining labels and their cytotoxicity effects at high concentration. *Nanotechnology* 19(41): 415102.
- Glazman, L.I. 2000. Single electron tunneling. *Journal for Low Temperature Physics* 118(5-6): 247-269.
- Gosh, C., Pal, S., Goswami, B. & Sharkar, P. 2005. Theoretical study on size-dependent properties of GaAs_n cluster. *Chemical Physics Letters* 407: 498-503.
- Gupta, R.K. & Saraf, V. 2009. Nanoelectronics: Tunneling current in DNA-single electron transistor. *Current Applied Physics* 9: S149-S152.
- Hanafi Ithnin, Ahmad Radzi M. Isa, Mohd Khalid Kasmin & Saeed, M.A. 2012. Study of electrostatic potential surface around bipyramidal GaAs quantum dot. *Digest Journal of Nanomaterials and Biostructures* 7(4): 1787-1791.
- Howes, M.J. & Morgan, D.V. 1985. *Gallium Arsenide: Materials, Devices, and Circuits*. New York: Wiley.
- Huffaker, D.L. & Deppe, D.G. 1998. Electro luminescent efficiency of 1.3 μm room temperature GaAs-based quantum dot. *Appl Phys. Lett.* 73: 2564-2565.
- Karamanis, P., Begue, D. & Pouchan, C. 2007. *Ab initio* finite field (hyper) polarizability computations on stoichiometric gallium arsenide clusters GaAs_n (n=2-9): *Journal of Chemical Physics* 127: 094706.
- Karatzter, P., Morgan, C.G. & Scheffler, M. 1998. Density functional theory studies on microscopic processes of GaAs Growth. *Progress in Surface Science* 59: 135-147.
- Kastner, M.A. 2000. The single electron transistor and artificial atoms. *Ann. Phys. (Leipzig)* 9(11-12): 885-894.
- Kirstaedter, N., Ledentsov, N.N., Grundmann, M., Bimberg, D., Ustinov, V.M., Ruvimov, S.S., Maximov, M.V., Kop'ev, P.S., Alferov, Z.I., Werner, P., Gosele, U. & Heydenreich, J. 1994. Low threshold, large *T₀* injection laser emission from (InGa)As quantum dots. *Electron. Lett.* 30: 1416.
- Kuroda K., Kuroda T., Watanabe K., Mano T., Kiddo G., Koguchi N. & Sakoda K. 2010. Distribution of exciton emission linewidth observed for GaAs quantum dots grown by droplet epitaxy. *Journal of Luminescence* 130: 2390-2393.
- Lee, S., Shin, D.W., Kim, W.M., Cheong, B., Lee, T.S., Lee, K.S. & Cho, S. 2006. Room temperature synthesized GaAs quantum dot embedded in SiO₂ composite film. *Thin Solid Films* 514: 296-301.
- Li, W.Z. & Huang, M.B. 2003. Equilibrium structures and hyperfine parameters of some fluorinated hydrocarbon radical cations: a DFT B3LYP and MP2 study. *Journal of Molecular Structure (Theochem)* 636(1-3): 71-79.
- Liu, H.C. 2003. Quantum infrared photo detector. *Opto-Electronics Rev.* 11(1): 1-5.
- Schmidt, M.W., Baldrige, K.K., Boatz, J.A., Elbert, S.T., Gordon, M.S., Jensen, J.H., Koseki, S., Matsunaga, N., Nguyen, K.A., Su, S., Windus, T.L., Dupuis, M. & Montgomery, J.A. 1993. General atomic and molecular electronic structure system. *Comput. Chem.* 14: 1347-1363.
- Schouteden, K., Vandamme, N., Janssens, E., Lievens, P. & Haesendonck, C.V. 2008. Confinement of surface state electrons in self-organized Co islands on Au(111). *New J. Phys.* 10: 043016.
- Stevens, W.J., Krauss, M., Basch, H. & Jasien Can, P.G. 1992. Relativistic compact effective potential and efficient, shared-exponent basis sets for the third-, fourth-, fifth-row atoms. *J. Chem. Phys.* 70: 612-630.
- Sugawara, M., Ebe, H., Hatori, N., Ishida, M., Arakawa, Y., Akiyama, T., Utsubo, K. & Nakata, Y. 2004. Theory of optical signal amplification and processing by quantum dot semiconductor optical amplifier. *Phys. Rev. B* 69: 235332.
- Sun, Y.L., Chen, X., Sun, L., Guo, X. & Lu, W. 2003. Nanoring structure and optical properties of Ga₈As₈. *Chemical Physics Letters* 381: 397-403.
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