Optimization Parameters and Some Electronic Properties of AlSb Diamondoids: A Density Function Theory Study

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Abstract

Density function theory with LSDA/3-21G basis set is used to investigate the optimization parameters such as (angles and bonds) and some electronic properties include (cohesive energy, energy gap and lattice constant) of AlSb at nano diamantine and different size of(Linear, Ring, Diamantine and Tetramantine). The results of the present work show that the angles of AlSbH nano molecule in range (96,21-126.05 Å) are near to standard angle of diamond (109.47 Å). Therefore, it is found that the cohesive energy for molecules of studied in decrease state with increase size but the energy gap decreased in gradually shape from (5.2-2.1eV) with increase of the number of atoms, that typical is on the lattice constant**.** It is finally shown that the size molecules has direct effect on electronic properties to material studied that can used this material in different applications and according to the purpose asked for.

Keywords: Nanomolecules, Diamond Structure(zb), Diamond Structure(zb), AlSb, DFT

1. Introduction

Nanocrystals (NCs) are group of atoms that form a cluster. They are bigger than molecules (~1 nm in diameter), but not as big as bulk matter. Although the physical and chemical characteristics of nanocrystals change, one of their big advantages over larger materials is that their size and surface can be exactly controlled and properties tuned like quantum dots (a type of nanocrystal) [1].

Surface atoms of the nanocrystals have different environments and then display different features. Nanocrystals have a large number of surface atoms compared to the bulk; therefore, the characteristics of surface atoms have more contributions towards their properties [2].

Nanocrystalline semiconductor aluminum antimonide (AlSb) has been intensively investigated in recent years, because they have many applications in optoelectronics devices including diodes, transistors, solid state lasers, and photovoltaic cells. The performance of these devices usually depends on the electronic and optical properties of the materials used [3].

Aluminum antimonide (AlSb) is a compound semiconductor with an indirect band gap and has the zinc-blende (zb) structure [4]. Most researchers pay attention to this object such as Mohammad and Katir-cioglu [5] studied the electronic band structure of AlSb nanoclusters and they found that the indirect band gap of AlSb is close to its experimental value, but the direct band gap has a small discrepancy with its experimental value. AlSb crystal is used in a multitude of device applications, including light-emitting diodes (LEDs), lasers, detectors, and communication devices [6].

Density function theory has been chosen in the present work rather than other methods because this method is very reliable with complex systems.

In this work were investigated the optimization and some electronic properties of AlSb nanocrystale by using DFT method with 3-21g basis with help Gaussian 9 program (computer software is capable of predicting many properties of molecules and reactions, including the molecular energies and structures) [7] to make the calculations.

2. Theory

Today density functional theory (DFT) is one of the most important tools for calculating the ground state properties of metals, semiconductors and insulators. (DFT) is a quantum mechanical method used in physics and chemistry to investigate the electronic structure of many-electron systems, in particular molecules based up on a strategy of modeling electron correlation via general functionals of the electron density [8]. DFT is among the most popular and versatile methods available in computational physics and computational chemistry.

The functional predecessor to density theory was the Thomas-Fermi model, developed by Thomas and Fermi in 1927. They calculated the energy of an atom by representing its kinetic energy as a functional of the electron density, combining this with the classical expressions for the nuclear-electron and electron-electron interactions, which can both also be represented in terms of the electron density [9].

In DFT, the main focus is not on the N-electron wave function $\Psi = (\vec{x}_1, \vec{x}_2, \ldots \vec{x}_N)$ and the associated Schrödinger equation, but instead it is on the much simpler electron density $\rho(r)$. The electron density is the number of electrons per unit volume for a given state. It is dependent only on three coordinates regardless of the number of electrons of the system.

Thus the number of electron N as a function to the density is [10]:

$$N = \int \rho(\vec{r}) d\vec{r} \qquad \ldots\ldots\ldots(1)$$

The fundamental concepts of DFT rely on the ground state energy and all other ground state electronic properties are uniquely determined by the electron density. Furthermore, the exact ground state of the system corresponds to the electronic density for minimal total energy.

3. Results and Discussion

In the present work, used Gaussian program to calculate the optimization parameters such as (angles and bonds). Figure(1) represented tooptimized atomic sites. These properties are showed in Table (1)and Table(2) represents the type and values of angles in (degree) between the atoms and bonds in (Å).Table(1) show variation in the values of the angles hat due to the different locations of these angles in the molecule in addition to the effect of the different neighboring atoms and size of molecule, which cause the power of interaction between them but all values of angles near of experiential data .Figure (2) shows physical parameters of AlSb (linear, ring, diamantine and

tetramantane) that include tetrahedral angles, Figure (3) show bond length. The stander value of tetrahedral angles (109.47 degrees [11]. In diamond and zincblende structures is indicated in the Figure (2). The average experimental value of Al-H bond length is 1.62 Å [12].Which is in excellent agreement with present calculated value 1.61 Å. Previous Sb-H bond theoretically calculated bond length is 1.74 Å [13]. Which is also in excellent match with our calculated value 1.72 Å . Both Figures show excellent agreement between theory and experiment.

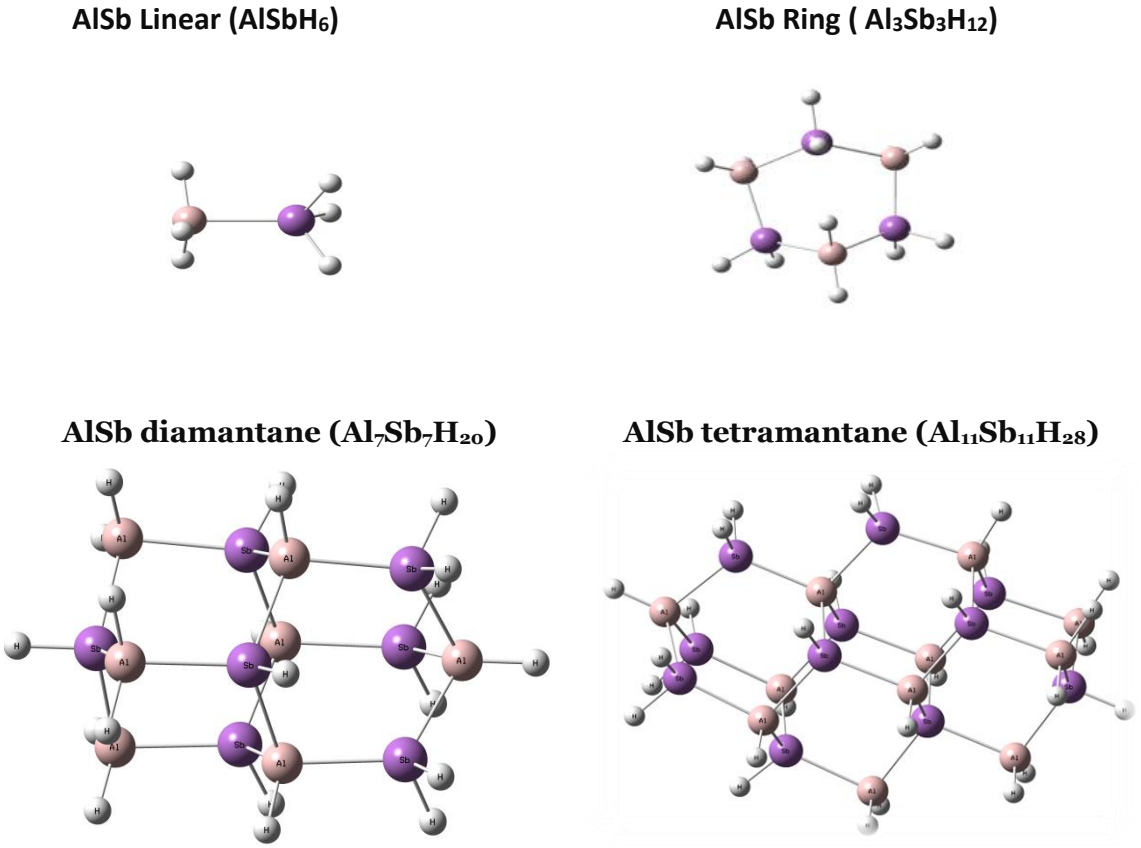


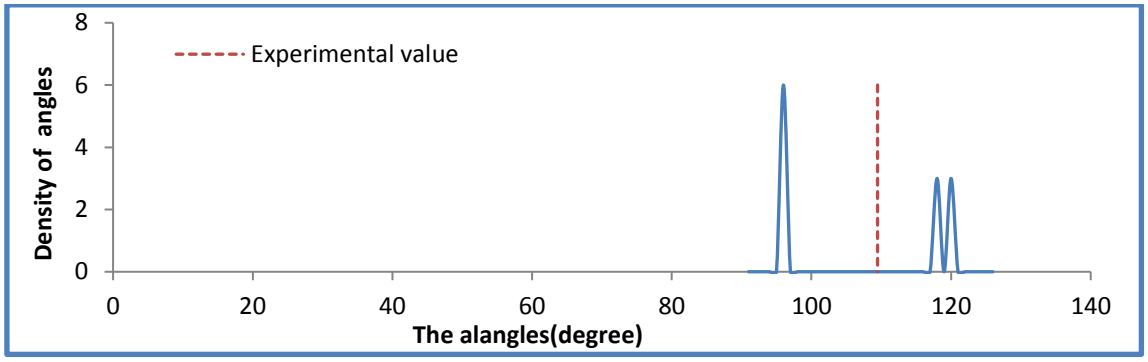
Figure (1): AlSb linear, ring, diamantine and tetramantane optimized atomic sites.

Table 1. The optimization parameters of AlSb nanocrystals (angles in degree)

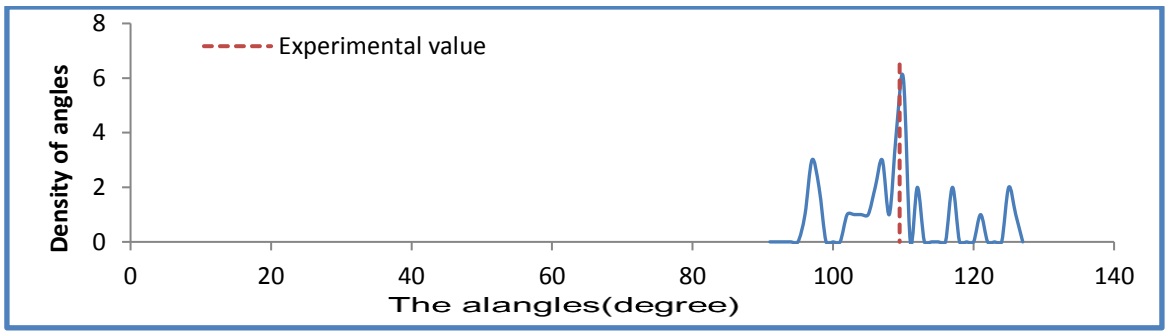
No. of bonds	The angles	Values in (Degree)
1	(Sb-Al-H)	96.212-1178675
2	(H-Al-H)	123.4894-126.0509
3	(Al-Sb-H)	101.4431-120.8454
4	(H-Sb-H)	97.7354-97.775
5	(Sb-Al-Sb)	96.43-110.5889
6	(Al-Sb-Al)	103.9867-121.6295
7	(H-Al-Sb)	110.8119-117.0077
8	(H-Sb-Al)	104.51-112.4086

Table 2. The optimization parameters of AlSb nanocrystals (bonds Å)

Name of Molecule	Chemical formula	The length of bonds	Values in (Å)
Linear	$AlSbH_6$	(Al-Sb)	2.7711
		(Al-H)	1.6232
		(Sb-H)	1.729
Ring	$Al_3Sb_3H_{12}$	(Al-Sb)	2.6952
		(Al-H)	1.615667
		(Sb-H)	1.72405
Diamantine	$Al_7Sb_7H_{20}$	(Al-Sb)	2.6771
		(Al-H)	1.616609
		(Sb-H)	1.7286
Tetramantine	$Al_{11}Sb_{11}H_{28}$	(Al-Sb)	2.6718
		(Al-H)	1.6167
		(Sb-H)	1.73023



Figure(2): Structural parameters of AlSb that include tetrahedral angles. Experimental value. The typical value of tetrahedral angles (109.47 degrees) [11]. In diamond and ZIncblende structures .



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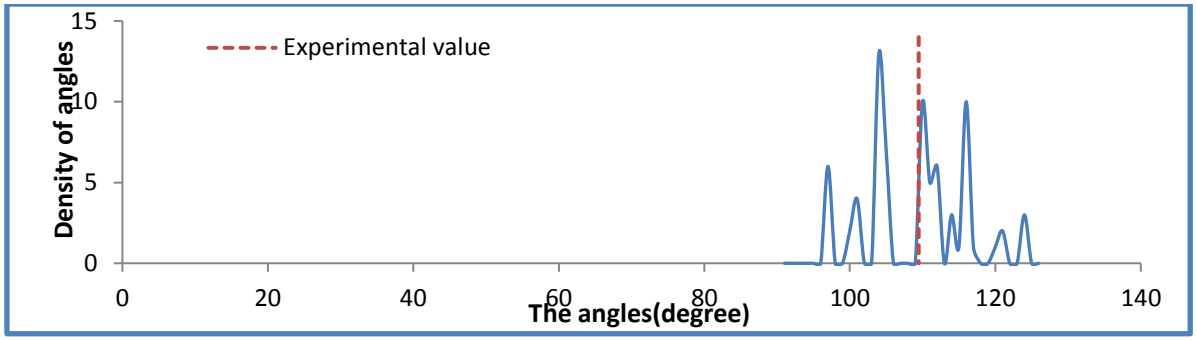

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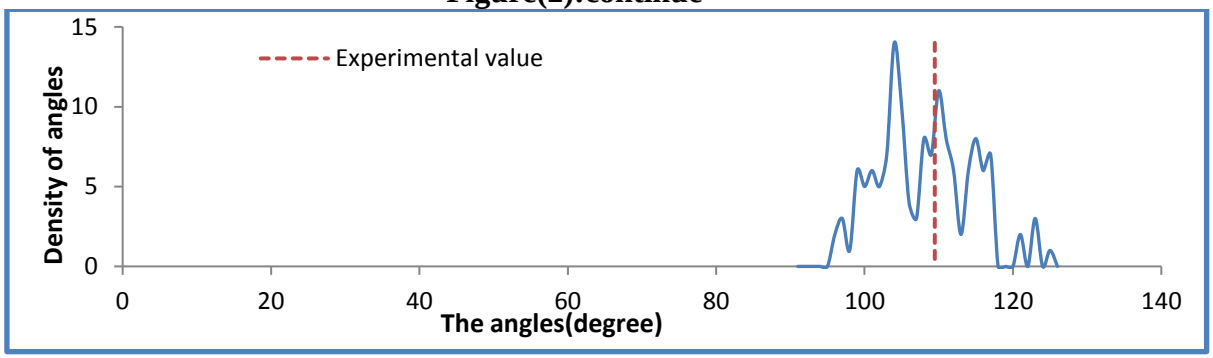

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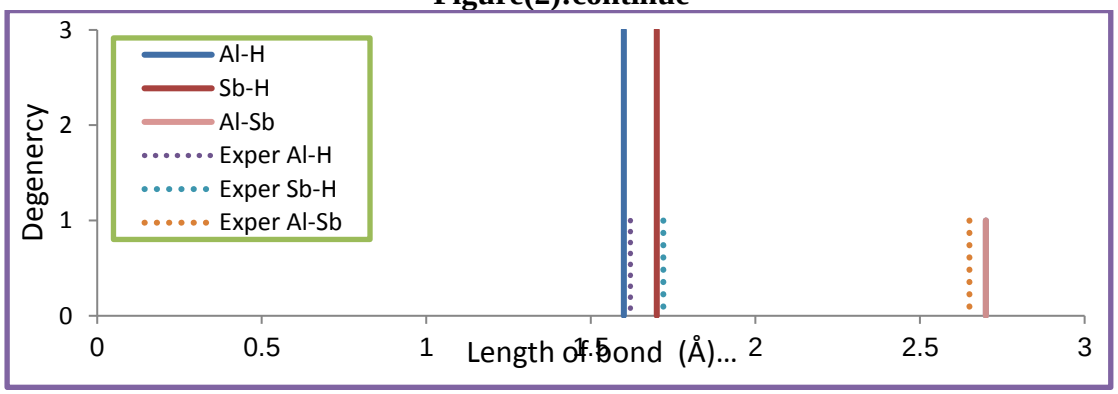
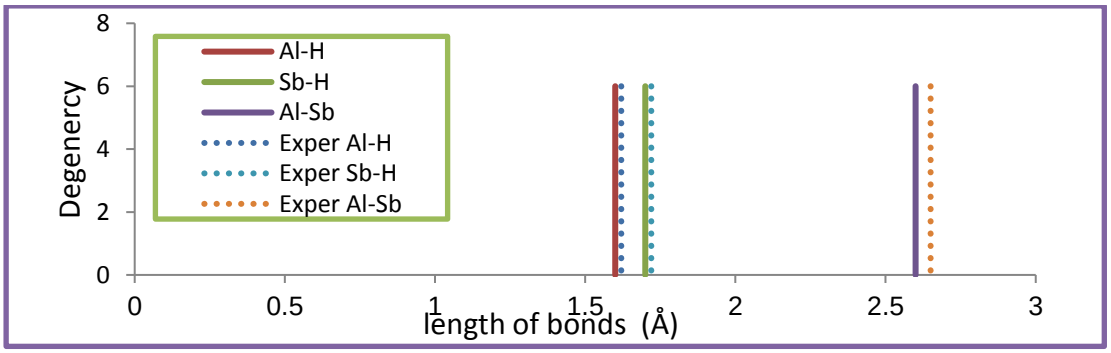


Figure (3): Structural parameters of AlSb that include bond length. Experimental value of (Al-Sb, Al-H and Sb-H) bonds length [13].



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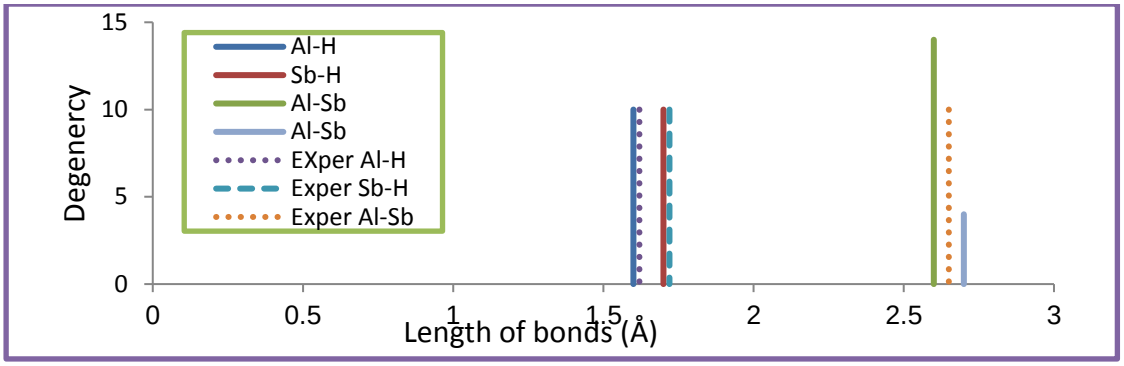

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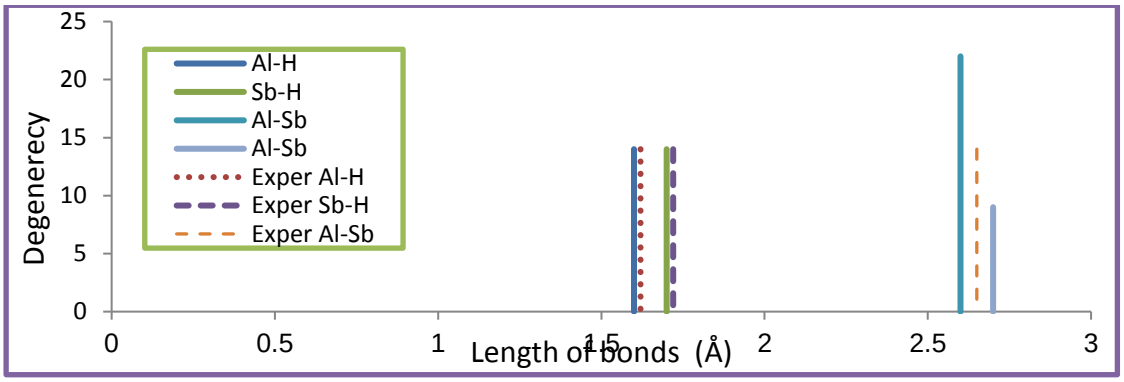

Figure (3): continue

Table(3): illustrates the results of (Cohesive energy, Energy gap and Lattice constant).Figure (4) show that the cohesive energy is decrease with increase the number of atoms in gradually shape nearly from experimental and theoretical data (8.08 and 6.60) respectively. Also, Figure (5) represented to the energy gap will start decreasing after increase size of diamond design of studies. Where the material behave the insulating material behavior and then gradually turn to the semiconductor material ,due to the effect of presence of the material in nonsocial dimensions which behaves contrary to all their individual molecular, therefore, Figure (6) shown that the lattice constant decreases with increasing the size of molecules.

4. Conclusion

LSDA/3-21G density functional theory has proved its validity in studying the geometry optimization and calculating the geometrical parameters with .

physical parameters of AlSb (linear, ring, diamantine and tetramantane) that include tetrahedral angles and bond length Both results show excellent agreement between theory and experimental value.

The present calculations show that the cohesive energy decreases as the AlSb molecule size increases (inverted relationship), and they tend to stabilize for nanocrystales of more than 50 atoms.

The present work exposes that the energy gap of AlSb nanocrystal for last structures equal to(2.19eV) is near of the experimental bulk AlSb crystal(1.68eV).

The lattice constant of all size of AlSb crystal decreased with increasing the number of atoms.

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الخلاصة

استخدمت نظرية دالية الكثافة ضمن المستوي LSDA مع الدالة الاساسG3–21 لفحص الامثلية الهندسية (الزوايا والاواصر) وبعض الخواص الالكترونية التي اشتملت على (طاقة الربط ,فجوة الطاقة والثابت الشبيكي) لجزيئة انتموناید الالمنيوم في الابعاد النانوية للجزيئات المدروسة باحجامها المختلفة المتمثلة في الجزيئات(الخطية, الحلقية, الثنائيمانتان, والثلاثيمانتان).

اظهرت النتائج ان قيم الزوايا الناتجة تتراوح بين(96.21–126.05 degrees) وكانت مقاربة للزاوية القياسية للجزيئات الماسية والتي تساوي (109.47 degrees) .

وكما اظهرت النتائج ان طاقة الربط للجزيئات المدروسة انها في حالة تناقص مع زيادة عدد الذرات وكذلك نقصان فجوة الطاقة بشكل تدريجي من (5.2–2.1eV) اقترابا من القيمة العملية المدروسة للمادة في حالتها الصلبة والتي تساوي (1.68eV) وهذا ما ينطبق على الثابت الشبكي ايضا.

مما سبق نستنتج ان للحجم الجزيئي النانوي تأثير مباشر على الخواص الالكترونية للمادة المدروسة وبالتالي ذلك مما يتيح امكانية استخدامه بالتطبيقات المختلفة وحسب الحاجة .

الكلمات المفتاحية: الجزيئات النانوية, التراكيب الماسية, انتيموناید الالمنيوم, نظرية دالية الكثافة.