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Theoretical Study ofthe Silicon 20 asa Quantum Dot

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Abstract:
The semi-empirical calculations of the electronic properties of silicon clusters as a function of oxygen position and other types of atoms are presented. The electronic properties of these clusters are calculated using PM3. We studied the dependence of the electronic properties on the number of oxygen atoms as well as on the geometric configuration of these clusters. The applied electric field showed the shifting in the electronic density distribution on the cluster.

Keywords: Silicon cluster, Quantum dot, PM3, Electric field.

1. Introduction

The study of silicon quantum dots is a very important field. The silicon quantum dots have physical properties and their applications are in advanced optoelectronic devices [1–4]. The theoretical interest focused on the prediction of the energy gap for a nanoparticle size. The theoretical calculations on silicon quantum dots are of a semi-empirical nature [5–7]. They are based on the knowledge of the electronic structure of bulk silicon. Silicon nanoparticles have been studied as fundamental building blocks for the bottom-up approach to construct nanoscale device structures [6]. Tight coupled silicon quantum dots are very important for quantum information device applications. The wave function interaction has been studied for double silicon quantum dots, which are the bonding-like and anti-bonding-like states, which have been observed at 4.2K [8]. Experimental studies have also been reported on the structures for small silicon quantum dots [9,10]. In the following section we describe our results on the methodology properties of silicon dots (Icosahedral structure). The ultimate goal is to artificially design and control the two level system and use as a quantum bit.

2. Computational Details

Theoretical calculations are used to bridge gaps in understanding the experimental results. In many cases the results of the experimental methods are unable to accurately describe small components or the nano-systems. The methods of molecular quantum mechanics can be used to investigate properties beyond the scope of current crystallographic methods. The molecular quantum mechanics provides the interaction energies that are not provided by the x-ray and NMR experiments [11]. The theoretical methods can be used to further investigation and to

predict the physical and chemical nature of nano-structure properties and their interactions. To investigate the structural and electronic properties of silicon quantum dots, we use PM3 (Parameterized Model number 3). PM3 is a semi-empirical SCF method for molecular calculations. PM3 is a reparameterization of the AM1 (Austin Model 1). PM3 and AM1 methods are generally the most accurate methods in HyperChem version. PM3 has been parameterized for many main group elements and some transition metals. The resolution of PM3 as implemented in the HyperChem™Release 7.52 for Windows Molecular Modeling System program package [12] was employed for the geometry optimizations.

3. Results and Discussion

3.1. Silicon Dot with Two Oxygen Atoms

In our calculations for Silicon nano-particles (Icosahedral structure) was represented by free-standing cluster, see figure 1. We considered nano-cluster with spherical shape, the number of silicon and hydrogen atoms ranging each. The semi-empirical calculations were carried out using PM3. We first performed Unrestricted Hartree-Fock (UHF) calculations to find the best geometry optimized the silicon clusters. Then we are doing single point calculations using Restricted Hartree-Fock (RHF).In the beginning, we focus on exchanging two hydrogen atoms by two oxygen atoms, so that we can make nano-quantum well, see figure 2. The question now, what to do to control on the width (w) and high (h) for this quantum well? We were postulating thatw was the distance between the two electronic densities, which ocalized at or near the double bonds between oxygen atoms and silicon cluster, while $h$was pointing to the activation energy between these two reigns. We studied the electronic properties of silicon clusters using Restricted Hartree-Fock (RHF) calculations. After performing geometry optimizations and calculating the highest occupied molecular orbitals as a function of the two oxygen positions on the silicon cluster, see figure 3. We can notice that the electronic densities are localized on or near the silicon-oxygen double bond, at the right and left sides of silicon cluster. The one oxygen atom changeits position toward the second oxygen atom, clockwise, where there are five issues, see figure 3, the fourth cause shown lowest total energy comparing with the other causes. The energy gap for these five causes shown increases as the positions of the two oxygen atoms approach. Especially, when the two oxygen atoms adjoin together, where the electronic density becomes more localizedapproximately in one side for the silicon cluster. If we consider that the force (F) on the silicon cluster as a function of surface area (S) and volume (V) at constant temperature can be approximately, $F^{Deformation} \sim SV$, then the forces on the silicon cluster shown the increases 7×10^{-5}, 29×10^{-5}, 10.9×10^{-3} and 10.68×10^{-3} as a function of the two oxygen positions on the silicon cluster respectively. This may be led to even decrease in silicon cluster volume or deformation in the silicon cluster shape as the two oxygen atoms closed to each other. We may conclude here that in the first case the electronic distribution bounded at two double bonds and as in the least case the electronic density bonded at one side through small region. The energy gaps as a function of the two oxygen positions on the silicon cluster are 2.288, 2.417, 3.096, 3.387 and 4.829 (eV), respectively.

Figure 1. The silicon cluster structure optimized using PM3. The silicon atoms are blue and the hydrogen atoms are white.

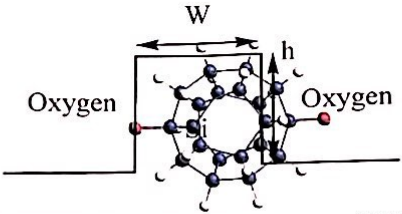
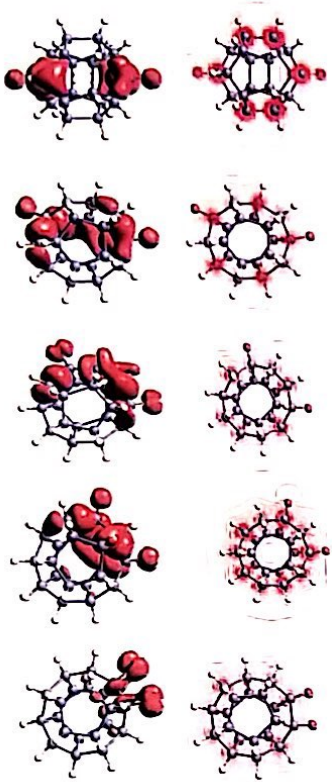


Figure 2.The scheme of nano-quantum well and silicon cluster with two oxygen atoms. The silicon atoms are blue, the hydrogen atoms are white and the oxygen atoms are red.

The present PM3 calculations show the increase in the energy gap (E_g) of silicon cluster as the oxygen atoms approach one from each other So that as the two oxygen atoms close to each other, the ionization energy (IP) for this system will increase, see figure 3 This result points out to the decrease in the ability of oxidation of this cluster Also the ability to capture the electron decreases due to the lowering in the electron affinity (EA) Figure 3 showed the electrostatic potential distribution of the silicon cluster with two oxygen atoms as a function of the two oxygen positions on the silicon cluster. In the first case their symmetric and more electrostatic potential intensity (EPI) at the two oxygen atoms, then this symmetry disappears and fluctuates in electrostatic field intensity The change in EPI may be able toconsideras high (h)for the quantum well, see figure 2, while the distance between the oxygen atoms as width (W)for the quantum well. We may conclude here that the change of the oxygen atoms position on cluster surface can be consider as tool todo control in the design of the quantum dots.



ΔE = +110 68 Kcal/mol
E_g = 2 288eV
ΔIP = 0 00eV
ΔEA = 1 096eV

ΔE = +112 04 Kcal/mol
E_g = 2 417eV
ΔIP = 0 126eV
ΔEA = 1 093eV

ΔE = +111 78 Kcal/mol
E_g = 3 096eV
ΔIP = 0 433eV
ΔEA = 0 721eV

ΔE = 0 0 Kcal/mol
E_g = 3 387eV
ΔIP = 0 70eV
ΔEA = 0 697eV

ΔE = +21 73 Kcal/mol
E_g = 4 829eV
ΔIP = 1 445eV
ΔEA = 0 00eV

Figure 3 the highest occupied molecular orbitals and the electrostatic potential distribution of the silicon cluster with two oxygen atoms as a function of the two oxygen positions on the silicon cluster using PM3.

3.2. Silicon Dot with Multi-atoms

We try to do more control to the quantum dot electronic properties by using two oxygen atoms at the left side of the silicon cluster and two oxygen atoms at the right side see figure 4 The operation of putting more distance between the two oxygen atoms showed more localized for the two electronic densities with gap between them more than the case when the two oxygen atoms become more

neighbored Also there is an increase in the force of deformation1 272×10^{-3} in the silicon cluster The silicon cluster with four oxygen atoms showed more energy gap as the space distance between the adjoined oxygen atoms at any side increases When the two oxygen atoms become more closed together, the ionization potential will increases and the oxidation will be more difficult with lower in the ability of capturing the vacuum electron The EPI shows ability of more control by using four oxygen atoms

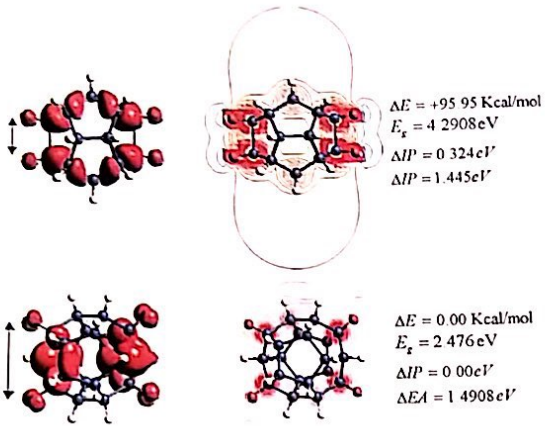


Figure 4. The highest occupied molecular orbitals and electrostatic potential distribution of the silicon cluster with four oxygen atoms using PM3.

3.3. Silicon Dot with Different Atom Type

We hypothesis the silicon cluster with two atoms from B, N, P, F and Cl atoms respectively, see figure 5 Table 1 shows the properties of silicon clusters as a function of exchange oxygen atom by B, N, P, F and Cl atoms respectively The silicon cluster with two phosphorus atom shows the lowest geometry deformation when compared with others also the case with two nitrogen atoms The phosphorus silicon cluster has the lowest energy gap and ionization potential when compare with the other issues, while it has highest electron affinity. In other word, it becomes good electron capture and difficult to ionize by other atoms The comparison of the highest occupied molecular orbitals of the silicon cluster with two different types of atom such as two boron atoms and phosphorus atoms shows best space localize to th electronic densities

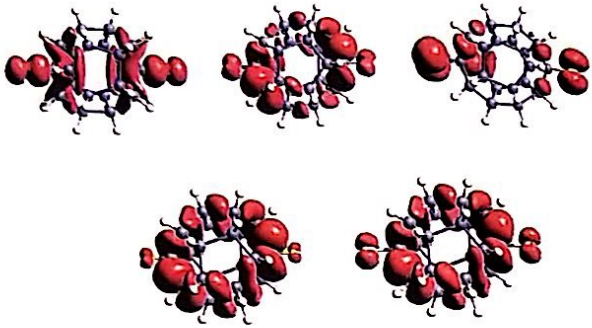


Figure 5. The highest occupied molecular orbitals of the silicon cluster with two atoms from B, N, P, F and Cl atoms, respectively by using PM3.

Table 1. The properties of silicon clusters as a function of exchange oxygen atom by B, N, P, F and Cl atoms respectively using PM3.

Atom	Eg (eV)	ΔIP (eV)	ΔEA (eV)	$F^{Deformation} \times 1000$
B	4 65	0 55	0 08	52 61
N	4 99	0 98	0 17	38 34
P	3 21	1 10	0 97	44 00
F	5 44	1 33	0 07	57 37
Cl	5 11	0 92	0 08	59 78

3.4. Applied Electric Fields

Figure 6 shows the influence of applying an external electric field parallel the major axis of silicon cluster which content the two oxygen atoms Dramatic increase in the high occupied molecular orbital distribution on the left side of silicon cluster while a decrease on the other as the electric field increase, which shows the ability of make control on the electronic densities. The operation of pushing the electronic distribution is fluctuated by applying very high electric field

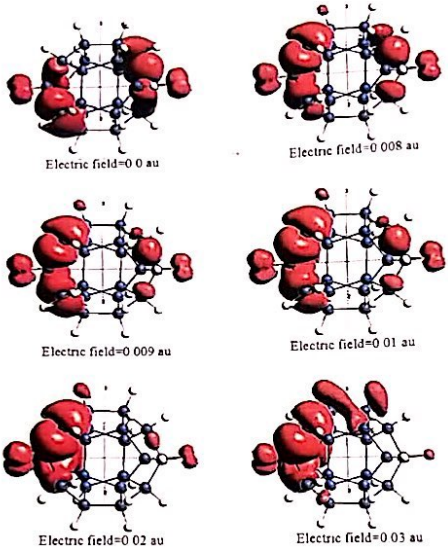


Figure 6 the influence of applied an external electric field in the major axis of silicon cluster with two oxygen atom.

4. Conclusions

Our results for the properties of silicon clusters show that the semi-empirical techniques are very useful tools to study the properties of quantum dots and to give good initial predictive information so that it can be used to interpret and complement experiments The position of the two oxygen atoms makes good control on the energy gap, stability, the deformation force and limited the oxidation and reduction processes Once we replace the two oxygen atoms, so this will give new properties and show another control Influence of applied external electric field showed shifting in the electronic density distribution toward the field

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دراسة نظرية للسيليكون 20 كنقطة كمية

سميرة فاخر رسن

قسم الفيزياء-كلية العلوم- جامعة البصرة-البصرة- العراق

الملخص:

تعرض حسابات شبه تجريبية للخصائص الإلكترونية لعناقد السيليكون كدالة لموقعذرة الأكسجين وذرات من نوع آخر. الخصائص الإلكترونية لهذه المجموعات تم حسابها باستخدامPM3. نناقش اعتماد الخصائص الإلكترونية على عدد ذرات الأكسجين وكذلك على التكوين الهندسي لهذه المجموعات. تسليط المجال الكهربائي أظهر التحول في توزيع الكثافة الإلكترونية.

المفاتيح: عناقد السيلكون، نقطة كمية،PM3، المجال الكهربائي