

# Ab Initio Calculations for the Effect of Pressure on the Structural Properties of Si Nanoclusters

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## ABSTRACT

Lattice constant, bulk modulus, Young modulus, valence band width, conduction band width, energy gap, vibrational energy, and plasmon energy have been calculated under compression and tensile stresses in the range ( $0 \pm 10$  GPa) for 8, 54, 128 atom clusters of silicon by means of density functional theory method with restricted Hartree-Fock theory within the framework of large unit cell approach. It is found that the results deduced from eight atom cluster are in good agreement with the corresponding experimental values. On the other hand, bulk modulus, young modulus, valence band width, energy gap, and Plasmon energy increase (decrease) under compression (tensile), while volume decreases (increases) with compression (tensile). The vibrational energy has a minimum value at the ground state point. The conduction band width has no systematic behavior with pressure.

**Keywords:** Nanocrystals; Pressure; Structural; Si

## 1. Introduction

Electronics is one of many interesting fields that IV materials can be implied in [1-6] so they have been subjected to extensive investigations [7-14]. Silicon, a very important semiconductor, is the principal component of most semiconductor devices; it is widely used in the semiconductors industry because it remains a semiconductor at higher temperatures than the semiconductor germanium, and because its native oxide forms a better semiconductor/dielectric interface than any other materials. The applications of silicon are in the electronic current conduction control (transistors), IC, detectors, solar cells and so forth. Nanocrystalline silicon (nc-Si) has small grains of crystalline silicon within the amorphous phase (a-Si). One of the most important advantages of nanocrystalline silicon is that it has increased stability over (a-Si) [15-20].

Understanding the properties of Si nanocrystals is an interesting field. Up to our knowledge, the effect of pressure on the properties of Si nanocrystals has not been comprehensively investigated. So the aim of the present work is to achieve this task.

Density functional theory (DFT) method in addition to Hartree-Fock (HF) theory within the Large unit cell (LUC) method [14] are used for calculating the total energy, lattice constant, bulk modulus ( $B$ ), Young modulus

( $Y$ ), valence band width (VBW), conduction band width (CBW), energy gap ( $E_g$ ), vibrational energy ( $F_{vib}$ ), and plasmon energy ( $E_{pl}$ ).

## 2. Method

The self-consistent Hartree-Fock method is used in the present work to obtain the electronic structure of silicon nanocrystals. Correlation corrections can be neglected in some closed-shell calculations (which is the case of the present work) using Koopmans theorem [21] owing to the cancellation of correlation corrections with relaxation. STO-3G basis states are used as the simplest basis to reach higher number of atoms [20,22-24].

Large unit cell (LUC) method coupled with *ab initio* Hartree-Fock self-consistent electronic structure calculations are used in the present work. LUC method was formulated and used previously to investigate the electronic of several kinds of bulk materials including diamond [20,23-25]. Semiempirical LUC calculations were performed previously for silicon nanocrystals [22] with smaller number of atoms. This method uses ( $k = 0$ ) approximation, that is one point in the wave vector space. The LUC method is one kind of supercell methods with the above  $k = 0$  restriction. In this method, and instead of adding more  $k$  points, the single central cell is expanded to contain more atoms, which are called core atoms in the present work. We found this method very suitable for

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describing the core of a nanocrystal since it still has the outer dangling bonds that are saturated by surface atoms. The method does not expand to contain the whole space; instead it contains only the real number of atoms in a nanocrystal core that has nearly the exact diamond structure [14]. Gaussian 03 program has been used for the present calculations [26].

### 3. Calculations

After the structure optimization, we calculate the lattice constant ( $a_0$ ), the cohesive energy ( $E_c$ ) and total energy ( $E_0$ ) in the ground state (zero temperature and 1 atmosphere). The cohesive energy is calculated from (Equation (17) in Ref. [27]). Results were fitted to Equation (1), the equation of state of Murnaghan, to estimate the change of energy with pressure  $E(V)$ , [28] and to determine the change of vibrational energy  $F_{vib}$  Equation (2) [29],

$$E(V) = E_0 + \frac{B_0 V}{B'_0} \left[ \frac{(V_0/V)^{B'_0}}{B'_0 - 1} + 1 \right] - \frac{B_0 V_0}{B'_0 - 1} \quad (1)$$

$$P_T = -\frac{\partial E(V)}{\partial V} - \frac{\partial F_{vib}}{\partial V} \quad (2)$$

where  $P_T$  is the isothermal pressure,  $V_0$  and  $B_0$  are the volume and the bulk modulus of the unit cell at the standard conditions and  $V$  is the volume at any pressure. The bulk modulus is calculated by Cohen empirical formula [30]:

$$B_0 = \frac{1970 - 200I}{d^{3.5}} \quad (3)$$

$I$  is the ionicity factor which equals 0, 1 and 2 for IV, III-V and II-V groups respectively [30],  $d$  is the interatomic distance [31]. Then the isothermal bulk modulus at any pressure ( $B_T$ ) has been calculated as [32]:

$$B_T = B_0 + B'_0 P_T \quad (4)$$

where ( $B'_0$ ) is the derivative of bulk modulus at zero pressure. The volume is calculated from:

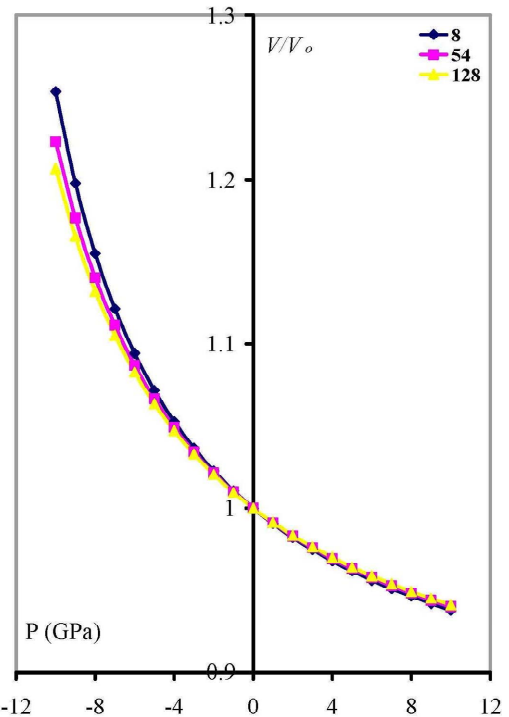
$$B_T = -V \frac{dP_T}{dV} \quad (5)$$

The results of pressure vs. volume ( $P-V_0/V$ ) relation are shown in **Figure 1**. On the other hand, the Young modulus is calculated from [33],

$$Y = \frac{P_T}{\varepsilon} \quad (6)$$

where  $\varepsilon$  is the strain. We have from Mijbil *et al.* [34] that the energy of plasmon ( $E_{pl}$ ) is:

$$E_{pl} \text{ (eV)} = 210.0563 \sqrt{\frac{\exp(\phi)}{V_0}} \quad (7)$$



**Figure 1.** The variation of volume with pressure.

**Table 1.** The structural properties of Si at (0 K and 1 atm), the dimensions are Å, GPa, eV for length, pressure, and energy respectively.

	Pres.			Theo.	Ref.	Exp.	Ref.
	8	54	128				
$a_0$	5.41	5.33	5.28	5.427 5.383	[35] [36]	5.4307 5.431	[35] [36]
$B_0$	100.232	105.597	109.139	87.99 95.9	[35] [36]	98 96 - 99.4	[37] [38]
$E_g$	2.74	3.29	3.52	3.5	[20]	3.44	[39]
$E_{pl}$	16.693	17.07	17.313	16.4 - 16.9	[40]	16	[40]
$B'_0$				3.828 4.153	[35] [36]	4.09 4.24	[35] [37]
$P_{max}$				11.7 11.95	[41] [42]	12.5	[42]
$E_{ZPV}$				0.065	[38]		

where  $\phi = P_T/B_T$ .

### 4. Results and Discussion

Our calculated structural properties at (0 K & 1 atm) compared with other results are shown in **Table 1**.

It is known that DFT underestimates the band gap [43] due to the discontinuity of the potential of exchange-correlation [44] which explains the difference between our results and the experimental data.

The compression stress increases the density and decreases volume due to the shrinkage of orbitals [45] as shown in **Figure 1**, and the distance between atoms [46], which entails an increment in the bond strength [47] and bulk modulus [48] (**Figure 2**) because the bulk modulus depends upon the density directly, and the young modulus which depends upon the bulk modulus [49], and vice versa for the tensile stress.

**Figure 3** shows an increment in the plasmon energy with compression and a reduction of it with tensile stress. Korniyushin has showed that the plasma affects the charge distribution and so the sound wave [50]. On the other hand, the phonon frequency affects the effective charge [51], which depends upon the charge distribution and determines the plasma frequency [52]. Compression stress, according to Sanjurjo, increases the effective charge for IV-IV materials and vice versa [51]. Meanwhile, the effective charge reduction, according to Burstein, decreases the plasmon frequency [52], and then one can find that our results are in good agreement with experiment [51] for the behavior of plasmon energy. The vibrational energy increases with both stresses.

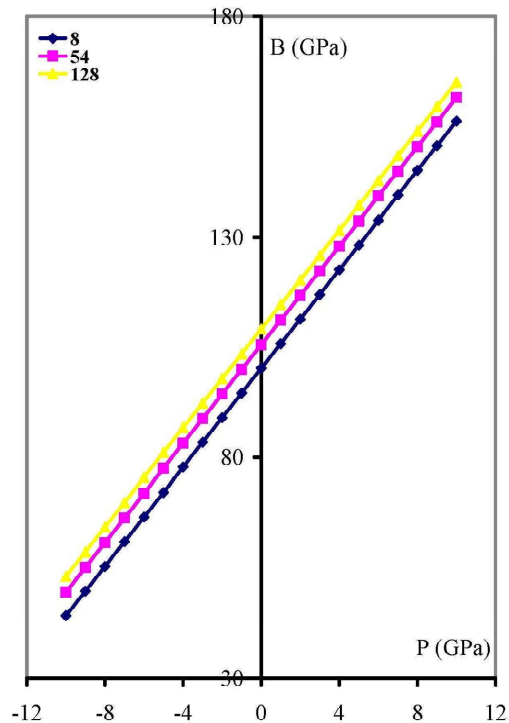
In order to get a further comprehension, the vibrational energy is considered. Its behavior is the same for all clusters and takes a minimum value at the standard conditions (0 K, 1 atm). It is known that atoms vibration is determined by phonons [53], and the velocity of sound depends on the atoms arrangement [54], while crystal is considered as a group of harmonic oscillators [55], according to Born-von Kármán theory. From all above and according to Polit who mentioned that the change of the lattice constant changes the charge distribution which affects the atoms' force field and these potentials modify the vibration energy [56]. On the other hand at zero temperature and according to Equation (2), the vibrational energy depends upon the behavior of the total energy which increases with stresses due to repulsion and attraction forces [57].

Energy gaps and valence band widths increase with compression, as shown in **Figures 4(a)** and **(b)** and they decrease with tensile stress, whereas the conduction band has no systematic behavior with pressure as shown in **Figure 4(c)**. It should be pointed out that increasing compressing means increasing overlapping and Coulomb interaction.

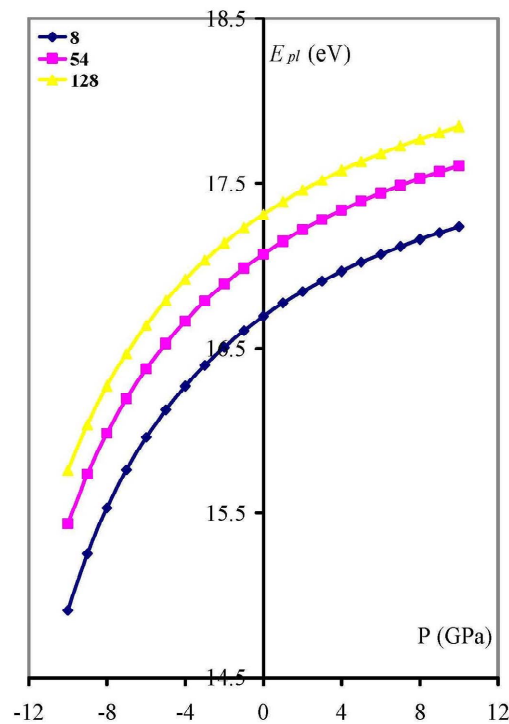
## 5. Conclusion

From the results of the present work, it shown that the density functional theory method with the restricted Hartree-Fock theory within the framework of large unit constitutes a powerful approach for investigating the structural properties of semiconductor nanoclusters. It is

found that the bulk modulus, Young modulus, valence band width, energy gap, and plasmon energy increase with compression, whereas the conduction band width has no systematic behavior with pressure. The conduction band



**Figure 2.** The variation of bulk modulus with pressure.



**Figure 3.** The variation of plasmon energy with pressure.

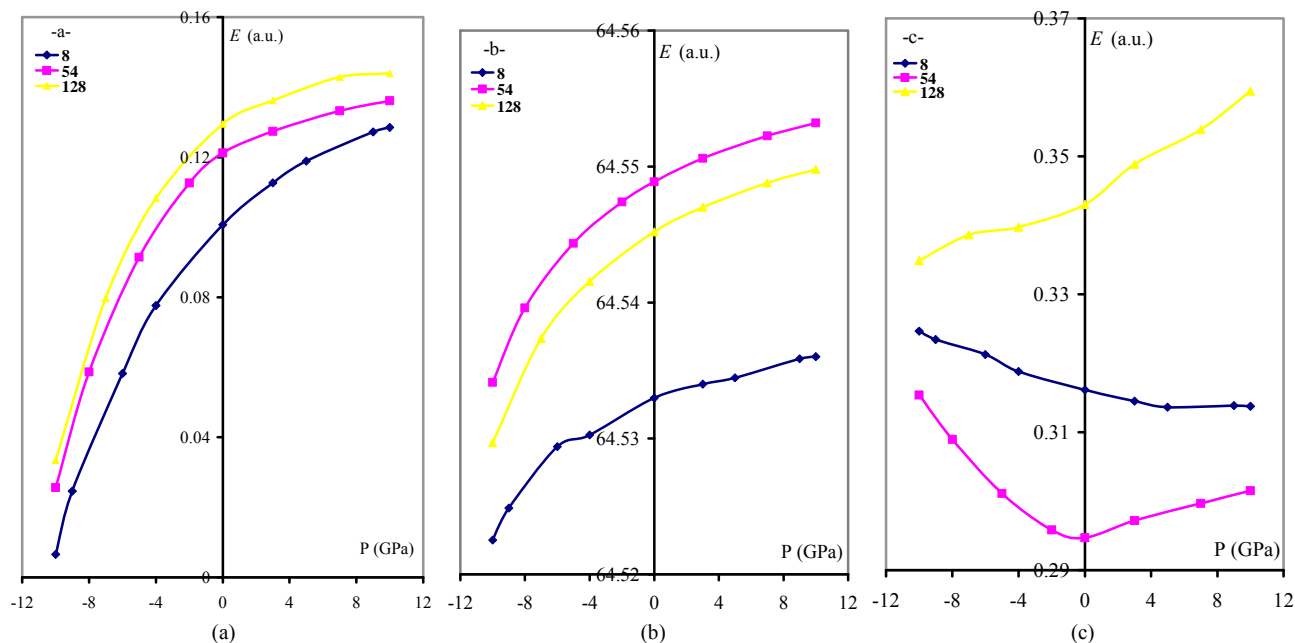


Figure 4. The effect of pressure on the: (a) Energy gap; (b) Valence band width; and (c) Conduction band width.

behavior needs more investigation, and it could be attributed to the different coulomb interactions and the delocalization of the  $p$  orbitals.

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