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Computational studies of planar, tubular and conical forms of silicon nanostructures

ABSTRACT

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Density functional theory (DFT) calculations were performed to investigate the properties of planar, tubular and conical forms of silicon nanostructures. The evaluated parameters including averaged bond lengths, binding energies, gap energies and dipole moments were then evaluated for the optimized models of study. The results indicated that the bond lengths between silicon atoms are different in the three forms of structures. The binding energies indicated that the planar form could be considered as the most stable form of silicon nanostructures among the investigated forms. Better conductivity of the conical form than the tubular and planar forms was confirmed by the gap energies. The dipole moments indicated that the planar and tubular forms of silicon nanostructures are non-polar whereas the conical form is a polar silicon nanostructure.

Keywords: Silicon, Nanostructure, Density Functional Theory (DFT), Nanosheet, Nanotube, Nanocone

INTRODUCTION

Since the days of carbon nanotube (CNT) discovery [1], considerable efforts have been dedicated to determine the applications and properties of this fascinating novel material [2,3]. Further efforts have also recognized the stable nanostructures other than CNTs and compositions of other atoms [4,5] as well. Among the new family of nanostructures, the silicon-based materials have attracted many attentions due to the similarities of the valance shells of carbon and silicon atoms [6]. Moreover, the tubular forms of silicon nanostructure have been reported by the computational and experimental investigations [7,8]. Rather than the tubular forms, the investigations indicated that the planar and conical forms are also available for the nanostructures. Indeed, the planar forms of nanostructures e.g., graphene, are so important that numerous researches have been so far performed in recent years to investigate their properties [9].

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The conical structures have been initially found as the caps of the tubular structures but soon turned out to be as free standing nanostructures [10]. The planar and conical forms of carbon nanostructures have been extensively investigated by the computational and experimental methods but the corresponding forms of silicon nanostructures have been rarely investigated.

In this work, we have performed density functional theory (DFT) calculations to investigate the properties of planar, tubular and conical forms of silicon nanostructures (Figure 1). To do so, we evaluated the structural properties for the investigated forms of silicon nanostructures through performing all-atomic geometrical optimizations. Apart from evaluating structural properties for each of the planar, tubular and conical forms, the obtained parameters could be also well compared among the mentioned silicon nanostructures.

COMPUTATIONAL DETAILS

Within this research, computations have been carried out at the DFT level employing the B3LYP exchange-correlation functional and the 6-31G* standard basis set using the Gaussian 98 package of program [11-14]. The models contain the main silicon (Si) atoms and the saturating hydrogen (H) atoms. Indeed, to avoid the dangling effects in the molecular calculations, the tips of

nanostructure are saturated by the hydrogen atoms [15]. It is important to note that the processing speeds of computers play as restricting factors for doing calculations; therefore, without high performance computational facilities, the models of this study have been chosen based on the available common computational facilities.

The representative planar form (Figure 1, panels a and d), which is a graphene-like nanosheet, contains fifty six Si atoms and twenty two H atoms. The representative tubular form (Figure 1, panels b and e), which is a (4,4) armchair nanotube, contains fifty six Si atoms and sixty H atoms. The representative conical form (Figure 1, panels c and f), which is a non cone with 240° declination angle, contains fifty eight Si atoms and fourteen H atoms. The all-atomic geometries of the investigated structures have been allowed to relax during the optimization processes. Subsequently the structural parameters of bond lengths, binding energies (E_b), gap energies (E_g), and dipole moments (D_m) have been evaluated in the optimized structures (Table 1). To evaluate the binding energy, the employed formula is $E_b = E[\text{Si}_x\text{H}_y] - E[\text{Si}] - E[\text{H}]$. To evaluate the gap energy, the employed formula is $E_g = E[\text{LUMO}] - E[\text{HOMO}]$, in which the formula designates the difference of energies between the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO).

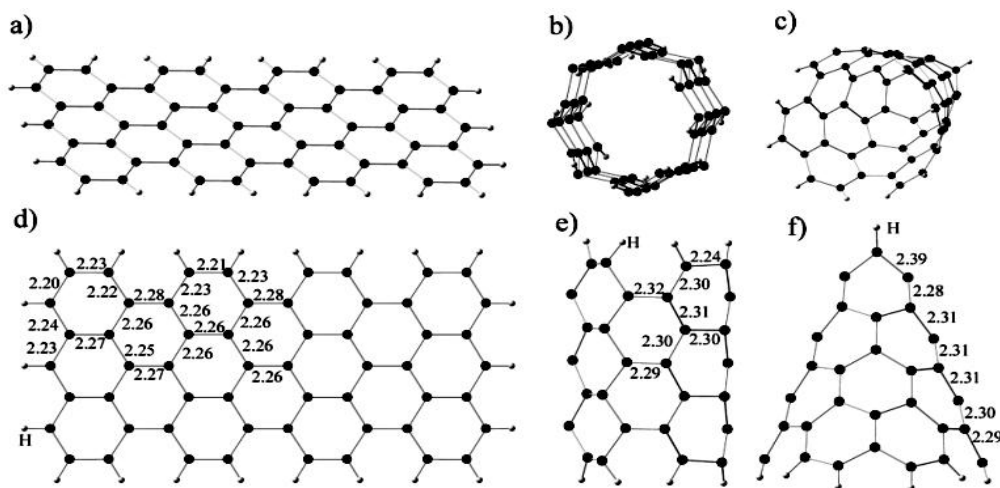


Fig.1. The planar (a and d), tubular (b and e) and conical (c and f) forms of the investigated silicon nanostructures. The upper row shows the 3D views and the bottom row shows the 2D views of the structures. The values of lengths are written on the selected bonds.

Table 1. The structural parameters of the optimized silicon nanostructures

Parameter	Planar Form	Tubular Form	Conical Form
Stoichiometry	Si ₅₆ H ₂₂	Si ₅₆ H ₁₆	Si ₅₈ H ₁₄
Averaged Si-Si Length /Å	2.25	2.29	2.31
Averaged Si-H Length /Å	1.48	1.50	1.49
Binding Energy /eV	-242	-226	-228
Gap Energy /eV	0.36	1.51	1.10
Dipole Moment /Debye	0	0	3.32

RESULTS AND DISCUSSION

The evaluated structural parameters including the values of average bond lengths, binding energies (E_b), gap energies (E_g) and dipole moments (D_m) are listed in Table 1 for the optimized Si nanostructures in planar, tubular and conical forms (Figure 1). The results indicate that the average values of Si-Si bond lengths are different in the investigated structures; the value for the planar form is the smallest and the value for the conical form is the largest. A quick look at Figure 1 indicates that the values of bond lengths are changed at the sites of the edges of the structures whereas the changes of the values in other sites of structures are negligible. The average values of Si-H bond lengths also exhibit small differences in the three investigated structures. The values of binding energies are important when it comes to compare the formation processes of the structures. The parameters for the three Si nanostructures indicate that the tubular and conical forms are almost similar with respect to the binding energies. However, the status of the planar form is significantly different from the tubular and conical forms. The values of binding energies indicate that the formation of planar form of Si nanostructure could be much more preferred than the tubular and conical forms. The conducting properties of structures could be detected by the values of gap energies, which are the differences between the HOMO and LUMO levels of energies. The larger value of gap energy refers to the lower conductivity and the smaller value refers to the higher conductivity of the structure. The results for the investigated Si nanostructures indicate that the

conductivity property of planar form is much more than the tubular and conical forms. Interestingly, the conical form exhibits better conductivity than the tubular form but all the three structures are considered to be as semi-conductors. It is known that the values of dipole moments refer to the polarizability of the structures. The results reveal that the values of dipole moments for planar and tubular forms are zero indicating that the mentioned Si nanostructures could be considered as non-polar structures. However, the non-zero value of dipole moment for the conical form refers to the polarizability of the conical form of Si nanostructure. Indeed, the evaluated parameters for the planar, tubular and conical forms of Si nanostructures reveal that different form of the Si nanostructures exhibit different behaviours, which are important in determining their applications for various purposes.

CONCLUSION

To investigate the properties of Si nanostructures, we performed DFT calculations on planar, tubular and conical forms of the Si nanostructures. The evaluated parameters indicated that the Si-Si bond lengths were changed in the three investigated forms; however, the changes of the Si-H bond lengths are almost negligible. The binding energies indicated that the formation process of the planar form could be preferred more than the tubular and conical forms. The values of gap energies indicated that the conductivity of planar form was much more than the tubular and conical forms. Moreover, the conductivity of

conical form was better than the tubular form. And as the final remark, the planar and tubular forms could be considered as non-polar Si nanostructures whereas the conical form could be considered as a polar Si nanostructure.

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