CHAPTER-2

Carbon-Silicon atomic chains Attached to Al-Electrodes

It is clear that whether or not a more complete description of the world is possible, those things that modern quantum theory does predict are predicted with incredible accuracy

- M.C. Payne

We report ab-initio calculations on synthesis and transmission co-efficient of 5-atoms and 7-atoms long atomic chains made of Carbon and Silicon. These chains are shown to be energetically favourable using bond strength calculations and structural relaxations. For transmission coefficient calculations chain is attached to Al electrodes on its both sides. Energetics and transmission coefficient have been computed using density functional approach implemented in plane wave based computer code PWSCF. Our computed results on transmission coefficients reported as a function of energy, which is measured from Fermi level, exhibit various peaks and dips for all chains and are nonzero for a wide energy range. The height, width and positions of these peaks change on replacing C-atoms by Si atoms. It is observed that value of transmission coefficient and range of energy having nonzero value of transmission coefficient enhanced on replacing C-atoms by Si-atoms. We find that transmission coefficient as a function of energy is determined by the ratio of Si to C atoms and the positioning of C and Si atoms in the chain. Behavior of T versus ε curve and magnitude of conductance values at the Fermi level highly depend on whether end-atoms in a chain are C-atoms or Si-atoms. The transmission co-efficient results obtained with the use of Al-bulk electrode provide wiggle free curves and they are found in qualitative agreement with the results obtained for Al nanorod electrode case.

2.1 Introduction

Recent progress in experimental techniques, such as the scanning tunneling microscope (STM), transmission electron microscope (TEM), mechanically controllable break junctions, atomic force microscopy (AFM), and high resolution transmission electron microscopy revolutionized the understanding of matter at its atomic level, not only due to the fact that they permit to image atoms, but also because some of them allow atomic manipulation [1-3]. They make it possible to study metallic nanochains, suspended between two electrodes, consisted of just a single metallic chain of few atoms or even one atom [4]. The fabrication of these atomic-size structures opens an intriguing prospect to discover a new physical phenomena and their technological usage, e.g. mmolecular electronics, which seeks to use individual molecules to perform functions in electronic circuitry, which are now performed by traditional semiconductor devices. Due to their potential use in molecular electronic devices and specially as nanocontacts, the electronic transport of Carbon (C) based nano-structures is one of the few fields that are immensely studied in last decade be it experimentally or theoretically/computationally. The variety of conditions in which CACs are formed, indicates that Carbon Atomic Chains (CACs) are preferential and stable at low density of C atoms. Recent discoveries [5-8] encourage to use the C atomic chain as interconnect between different devices of the nano circuitry entirely based on low dimensional C structures. Ijima and Chuvilin groups have derived linear CACs from single sheet of graphene using TEM and observed them highly stable even in presence of continuous energy input from the electron beam. Monatomic Carbon chains and chains consisting C and metallic atoms are well studied structures in past and also in recent. They show very promising characteristics regarding their use in nanodevices and especially as nanocontacts [9-15]. During their experiment Jin et al and Chuvilin et al observed that the chain never broke from middle and always from end when atomic chain was joined to

graphene. It would be interesting to study effect of Si, the base material of present day's micro-electronics and C, the promising candidate for future's molecular electronics on conductance at the atomic level. Chelikowsky et al had reported earlier that the Si atoms at the two ends of the nanotube can form stronger covalent linkage to electrode leads than metallic chain and therefore provide more accurate control over the contact geometry [16]. Moreover, due to advances in the miniaturization of electronic devices SiC nanowires have been used as building blocks. The electrical measurements from nanowire based FET structure show that SiC nanowires are intrinsic n-type semiconductor [17] and may be used in electric composites as reinforcement nanomaterial or in nanoscale electronic/ photoelectric devices under harsh environment [18]. It has also been observed in past that the infinite linear chain of the SiC is a good insulator. Effect of substituting C in 6 atom long Si chain has been found to decrease the conductance of Si chain [8]. However, there exists no thorough study of various atomic chains consisting of varying number of Si and C atoms. It will also be important to study such atomic constrictions made from C and Si due to their fundamental physical issue of how the valancy and different atomic orbitals of different atoms contribute to various properties of these low dimensional structures as both C and Si are isovalent. We have conducted a comprehensive simulation of the electronic and transport properties of various CACs, with the focus on dependence of Transmission coefficient on positions and numbers of C and Si atoms in 5 and 7 atom chains. It is common knowledge that linear carbon chains with fewer than ten atoms are thermodynamically more favourable than ring isomers, except for a C6 chain, which has degenerate linear and ring isomers in zero electric field[19]. It is well understood at nano scale that the chemistry and geometry of the scatterer both affect the electronic conduction.

Objective of this work have been two fold. Whether replacement of some Si atoms in C chain is energetically feasible and how does conductivity change on; (i) replacing C atoms by Si

atoms, (ii) varying the number of C and Si atoms and (iii) interchanging the positions of C and Si atoms in a chain of fixed atoms. The ab-initio calculations of synthesis and Transmission co-efficient of 5-atom and 7-atom chains having varying number of C and Si atoms have been performed. In addition, we have also investigated the difference in transmission of electrons through atomic chains when they are attached to Al bulk instead of Al nanorod.

2.2 Synthesis of atomic chains

We have performed first-principle plane wave calculations within DFT using well tested norm-conserving pseudopotentials [20] implemented in PWSCF code of Quantum Espresso package [21]. The exchange-correlation potential has been approximated by Perdew and Zunger formula for LDA. Following electronic states are treated as valance states for, Al ($3S^2$ $3P^1$); Si ($3S^2$ $3P^2$) and C ($2S^2$ $2P^2$). For partial occupancies, we use the Methfessel-Paxton smearing method. The energy smearing parameter near Fermi energy (E_f) was chosen to be 0.01 Ry. The energy cutoff of 35 Ry for wave functions has been used.

We computed the energetics of the synthesis of 5-atom and 7-atom chains of different combinations of Si and C atoms. These are; C-C-Si-C-C, C-Si-C-Si-C, Si-Si-C-Si-Si, Si-C-Si-C-Si, C-C-C-Si-C-C-C and C-C-Si-C-Si-C-C. We started from two atom configuration and relaxed it. Then third atom coming in sequence is brought near to two atom chain from infinite distance. At equilibrium bond length distance the three-atom system reaches to its minimum energy. If the energy of system when third atom is at infinite distance is set to zero, at bond-length distance, energy of system gives binding energy of third atom. The computed binding energy per atom is found to be in the range of -3 to -10 eV which shows that process is exothermic and synthesis is quite possible [22]. Further, we relaxed the three-atom chain to have maximum force per atom at 0.001 Ry and then the procedure is repeated for bringing other atoms from infinite distance. It is shown in Fig 2.1(a) by pictures taken from virtual atomic visualizing package Xcrysden [23]. This has been our method for synthesizing different atomic chains made of C and Si atoms. The energetics of different chains is displayed in Fig 2.1(a) to 2.1(f). The computed energetics of growth clearly demonstrates that the C-C-Si-C-C, C-Si-C-Si-C, Si-Si-C-Si-Si, Si-C-Si-C-Si, C-C-C-Si-C-C-C and C-C-Si-C-Si-C-C chains are not simply a theoretical construct of fundamental interest, but they can be realized experimentally.

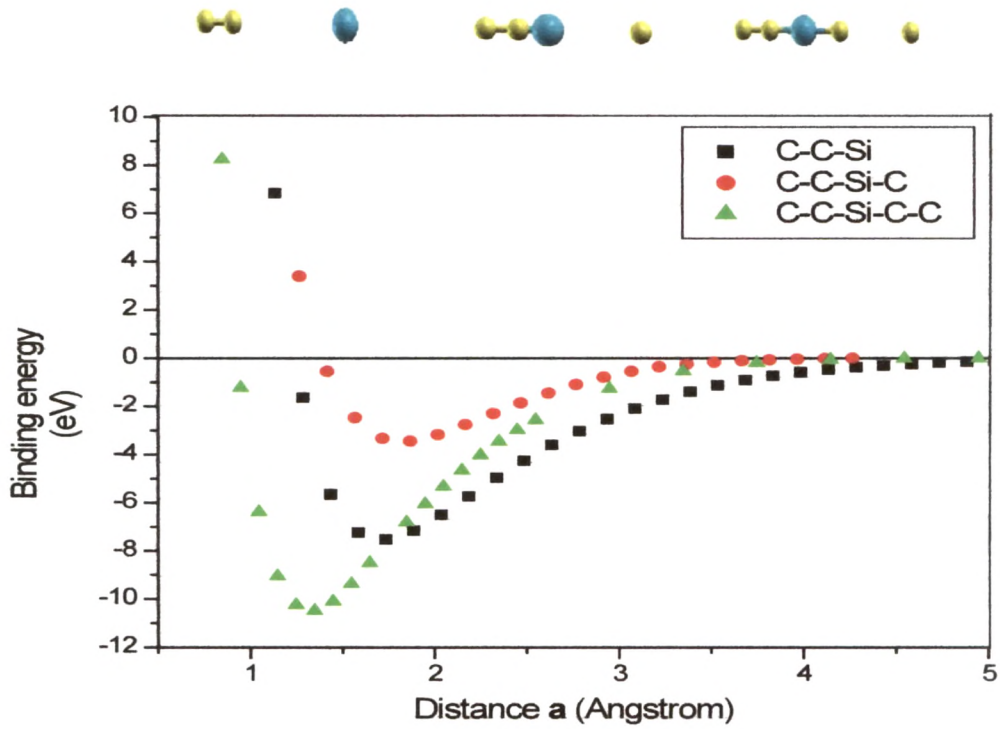

Figure 2.1 (a): Plot of binding energy per atom as a function of **a** (distance of the last added atom from the end atom of chain already in minimum energy configuration) for the formation of C-C-Si-C-C chain. The total energy of the system for $a \rightarrow \infty$ is set to zero for each curve.

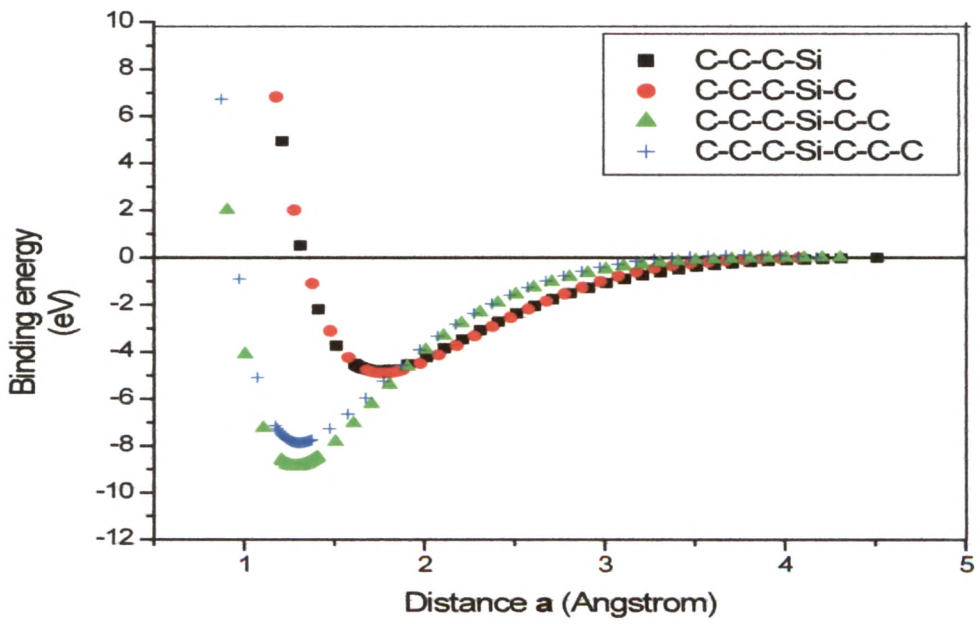

Figure 2.1 (b): Same as Fig. 1(a) for C-C-C-Si-C-C-C chain

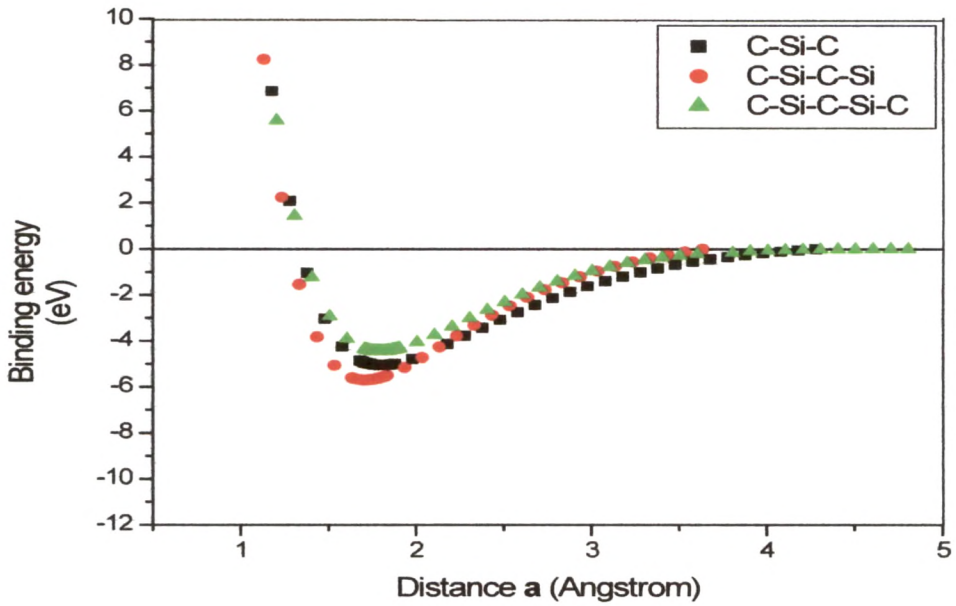

Figure 2.1 (c): Same as Fig. 1(a) for C-Si-C-Si-C chain.

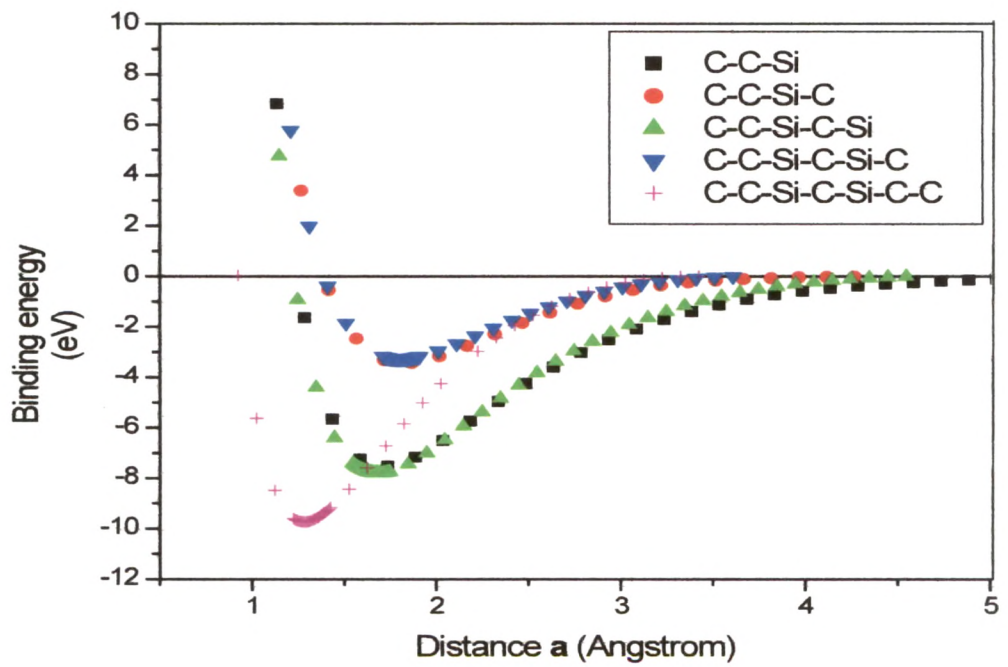

Figure 2.1 (d): Same as Fig. 1(a) for C-C-Si-C-Si-C-C chain.

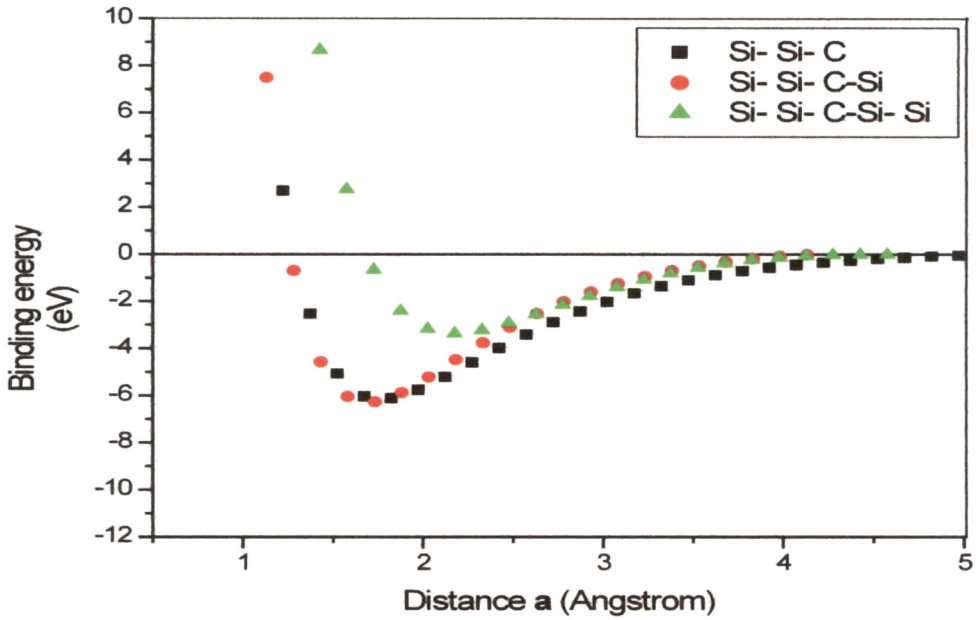

Figure 2.1 (e): Same as Fig. 1(a) for Si-Si-C-Si-Si chain.

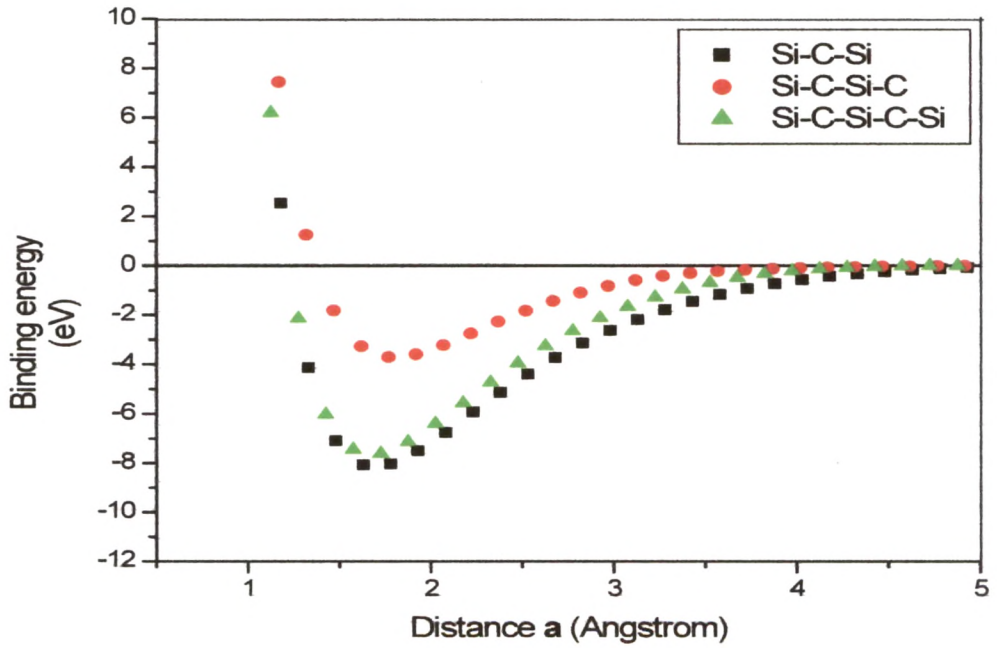

Figure 2.1 (f): Same as Fig. 1(a) for Si-C-Si-C-Si chain.

2.3 Transmission co-efficient calculations

After checking feasibility of atomic chains made of C and Si and synthesizing them, we computed transmission co-efficient of these atomic chains attached to Al electrodes. Together with checking the chemistry dependence of electronic transport through atomic chains our prime concern is to study also the effects of electrode size on the electronic transport. So we can divide our work reported in this chapter in two parts:

1. Atomic chains made of C and Si attached to ***Al nanorod*** electrode

2. Atomic chains made of C and Si attached to ***Al Bulk*** electrode

2.3.1 Si-C atomic chain Attached to Al nanorod

2.3.1.1 Computational Details

The supercell geometry consists of an atomic chain along with 4 layers of left electrode and 3 layers of right electrode. The size of supercell is made such that, in *x-y* plane periodically repeated structures are sufficiently far away (~9.18 Å) to prevent the interaction with adjacent replicas, while the structure is repeated in *z*- direction. Typical Supercell geometry is shown in Fig. 2.2 (a). The ab-initio calculation of ballistic conductance for carbon linear chain with 4-7 carbon atoms attached to Al-electrodes has also been performed in past using ultrasoft pseudopotentials [22, 24]. In order to verify the correctness of our methodology, we too first constructed carbon linear chain with 4 and 7 carbon atoms and placed them between two crystalline Al electrodes and optimized the geometry. Our calculation reproduces the previously reported results on transmission co-efficient for 4 and 7 carbon atom linear chains [24].

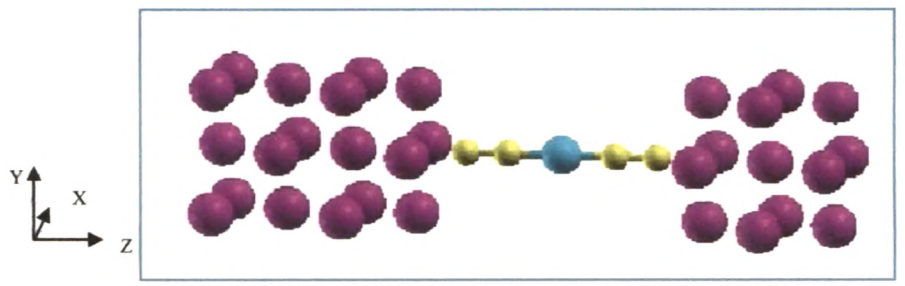

Figure 2.2 (a): A typical supercell consisting of C-C-Si-C-C chain attached to Al electrode oriented along (100) direction. C- Yellow, Si- blue and Al- pink spheres.

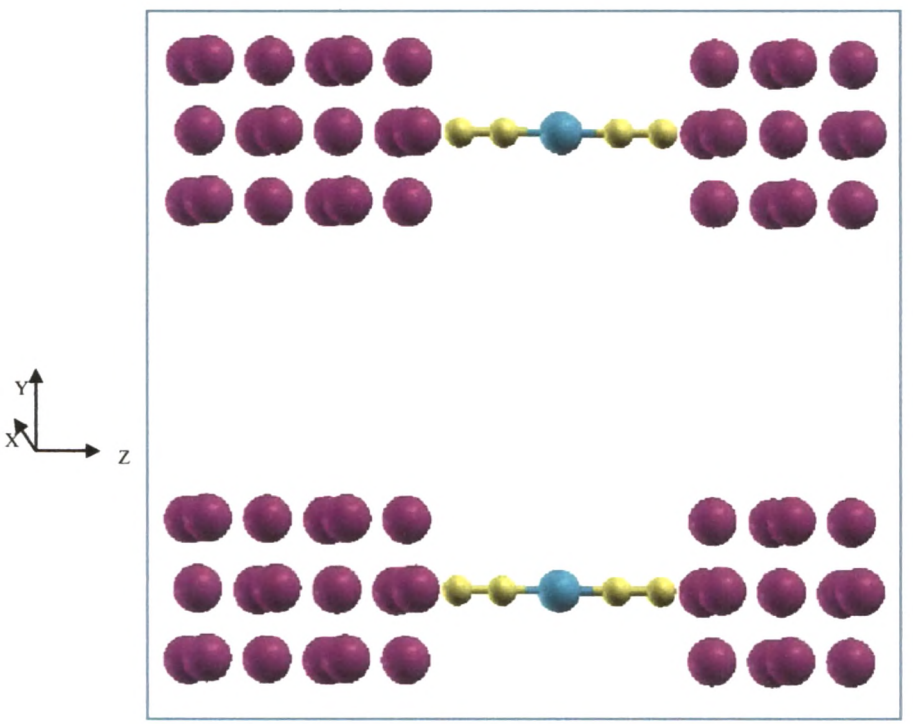

Figure 2.2 (b): A typical electrode-chain-electrode system and its periodic image formed in the *y* direction. Large vacuum of more than 9 Å is kept between system and its replica created. Similar replicas are formed in *x* direction also (not shown here).

We have relaxed the chains such that force between their constituent atoms is in the range of 10^{-3} Ry/au and then placed these relaxed chain between two semi-infinite Al-electrodes. The distance of last atom of chain from Al-electrodes is optimized to give minimum total energy. In the minimum energy configuration, the distances between Al-electrode surface and the last atom of chain on both left and right sides have been found to be; 0.95 Å for C-C-Si-C-C, 0.90 Å for C-C-C-Si-C-C-C , 1.00 Å for C-C-C-C-C, C-Si-C-Si-C, C-C-C-C-C-C and C-C-Si-C-Si-C-C chains, 1.4 Å for Si-Si-Si-Si-Si chain, 1.45 Å for Si-Si-C-Si-Si chain and 1.5 Å for Si-C-Si-C-Si chain. The sequence of computed equilibrium bond lengths in different chains are; 1.29, 1.67, 1.67, 1.29 Å for C-C-Si-C-C chain, 1.34, 1.32, 1.67, 1.67, 1.32, 1.34 Å for C-C-C-Si-C-C-C chain, 1.78, 1.70, 1.70, 1.78 Å for C-Si-C-Si-C chain, 1.32, 1.68, 1.65, 1.65, 1.68, 1.32 Å for C-C-Si-C-Si-C-C chain, 2.17, 1.69, 1.69, 2.17 Å for Si-Si-C-Si-Si chain, 1.67, 1.67, 1.67, 1.67 Å for Si-C-Si-C-Si chain and 2.14, 2.13, 2.13, 2.14 Å for Si-Si-Si-Si-Si chain.

The Al leads are simulated by a planar slab consisting of seven atomic (001) crystalline planes. Atoms of these seven layer slab are located at their ideal bulk FCC positions (with inter atomic spacing of 2.86 Å). The electrode unit cell made of two layers consisting of 9 atoms. The electrode layers on both sides of chain are useful to match the boundary conditions. The C, Si and Al atoms are described by well tested norm-conserving pseudopotentials [20]. The Brillouin zone has been sampled by special k-points generated using Monkhorst-Pack scheme [25]. The k-point sampling is done specially along z-axis due to 1D nature of scattering region. The size of supercell in x-y plane is chosen to be L_x=L_y=25 au ≈ 13.23 Å.

2.3.1.2 Results and Discussion

Our computed transmission coefficient, T for 5-atom chains are plotted in Figs. 2.3 (a) and 2.3 (b) and for 7-atom chains it is plotted in Fig. 2.3 (c), as a function of energy (ε) measured from Fermi level E_f, which is set to zero. As our lead-chain-lead system is non-magnetic, reported transmission co-efficient has been computed for per spin channel. The total transmission co-efficient can be obtained by doubling the values of T, displayed in Fig. 2.3(a) to 2.3 (c).

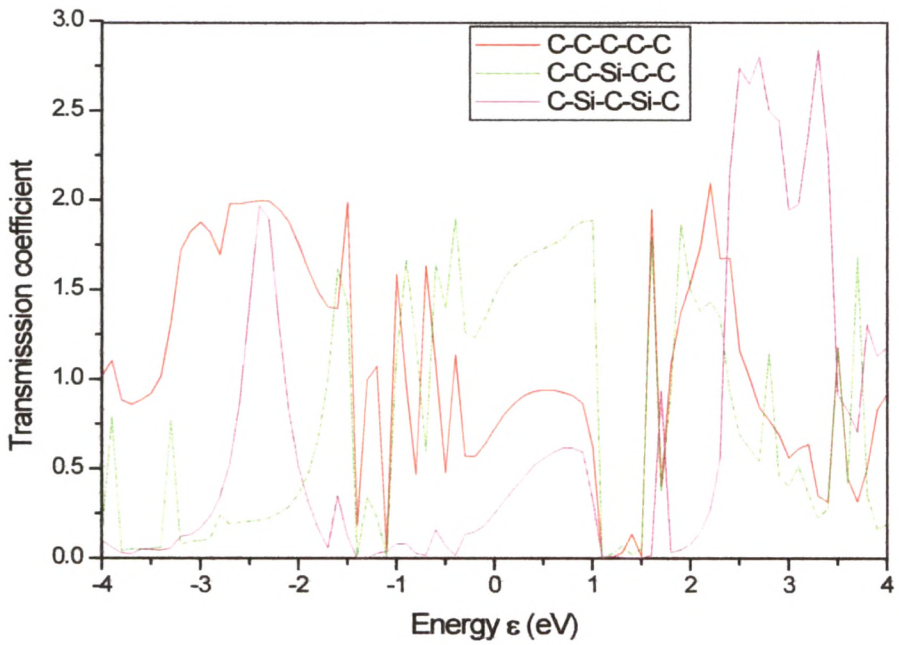

Figure 2.3 (a): Transmission Co-efficient T as a function of ε, energy measured from Fermi level for C-C-C-C-C chain, C-C-Si-C-C chain and C-Si-C-Si-C chain.

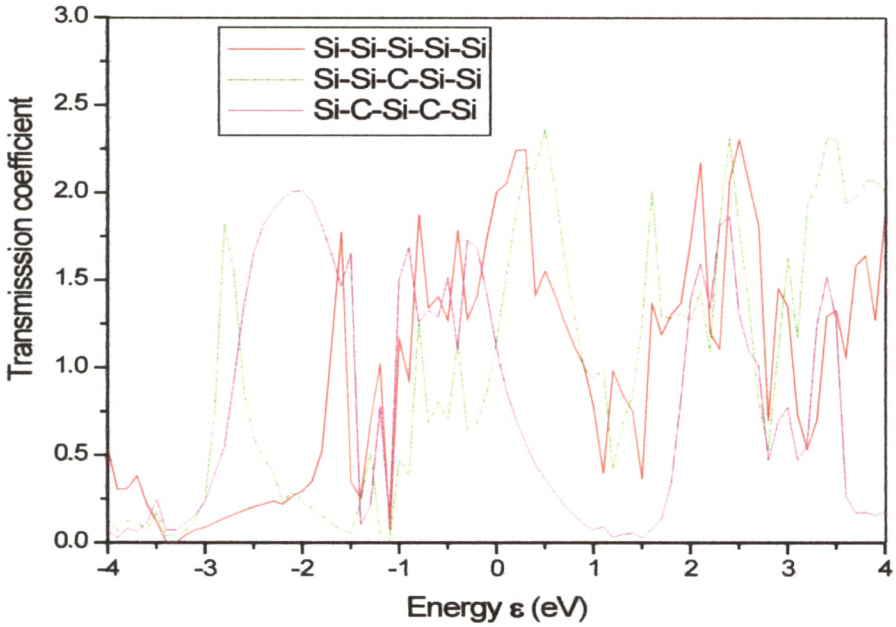

Figure 2.3 (b): Transmission Co-efficient T as a function of ε, energy measured from Fermi level for Si- Si- Si- Si- Si chain, Si- Si- C-Si- Si chain, Si- C-Si- C-Si chain.

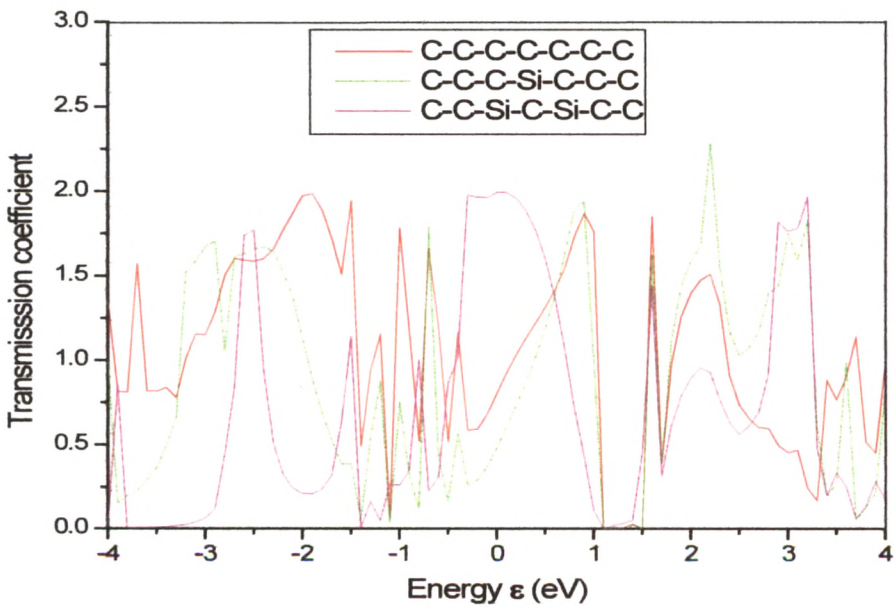

Figure 2.3 (c): Transmission Co-efficient T as a function of ε, energy measured from Fermi level for C-C-C-C-C-C-C chain, C-C-C-Si-C-C-C chain, C-C-Si-C-Si-C-C chain.

For all chains, we computed T for ε range of $E_f \pm 4$ (eV). Our computed results can be divided in three regions of ε; 4 to 1.5 eV, 1.5 to -1.5 eV and -1.5 to -4 eV. We term these energy regions as A, B and C, respectively. Intermixing of $3S^2\ 3P^2$ and $2S^2\ 2P^2$ orbitals on varying the number of Si and C atoms offers changed complex band structure of the chain. This results in a changed behavior of T as a function of ε. Looking at Figs. 2.3(a) to 2.3(c), we notice that the height of peaks, depth of dips, width and positions of both peaks and dips and the number of peaks and dips keep on changing, on replacing C atoms by Si atoms. The widest energy range of $-3.5\ \text{eV} \leq \varepsilon \leq 4.0\ \text{eV}$ that offer nonzero value of T is observed in 5-atom Si-chain. Our computed results on T exhibit that there are wiggles in the behavior of T as a function of ε in the range of 0 to -2 eV for all atomic chains. As can be seen from the Figs. 2.3(a) to 2.3(c), T for all atomic chains attains minimum value, almost zero in some cases, in the short intervals of energy around -1 eV and for energy values just above 1 eV. The computed results for 5 C-atoms chain suggest that all three regions are more or less equally open for transmission exhibiting largest value of T in the C-region. When middle C-atom is replaced by Si-atom to make C-C-Si-C-C chain, we get major changes in the behavior of T as compared to that of 5 C-atoms chain, as is seen in Fig. 2.3(a). Energy width of C-region is narrowed and it displays minimum value of T. The highest T-value for C-C-Si-C-C chain appears in B-region which is around Fermi level. However, the T remains more or less unchanged in energy A-region.

On comparing curves in Fig. 2.3(a), we find that on replacing second C-atom by a Si-atom to form C-Si-C-Si-C chain, the T-value drastically goes down in B-region. A and C-regions become better conducting regions displaying maximum T-value in A-region. The figure also suggests that replacing second C-atom by Si-atom shifts the maximum T by roughly 2 eV towards the higher ε-value. At the same time, regions having lower values of T are significantly suppressed. This can be understood in terms of change in complex band

structure and density of states on replacing C-atom by a Si-atom in a chain. The energy bands which were allowed for transmission become forbidden and forbidden turns to allowed, on replacing a C-atom by a Si-atom. Replacing another C-atom with Si-atom to form Si-C-Si-C-Si chain displays all together different behavior of T versus ε curve as compared to that for C-Si-C-Si-C chain. This is because of Si face the Al-electrode surface in the Si-C-Si-C-Si chain. The overall behavior of T versus ε curve for Si-C-Si-C-Si chain is somewhat similar to that of C-C-C-C-C chain. In Si-C-Si-C-Si chain all three regions offer very good values of T. The 5 Si-atoms chain and the 5 atom chain with only one C-atom at centre exhibit almost identical behavior except shifting of the peak from -3.0 eV for Si-Si-C-Si-Si chain to -2.0 eV for Si-Si-Si-Si-Si chain and the removal of wiggles in energy range of 0 eV to -1.0 eV. Similar changes in T versus ε curve are not observed when central C-atom is replaced by Si-atom in C-C-C-C-C chain to form C-C-Si-C-C chain. However, drastic changes in peak heights and positions were observed in this case. We thus can conclude that the replacement of a C-atom by Si-atom in 5 C-atoms chain brings much more drastic changes in T versus ε curve as compared to that on replacing one Si-atom by C-atom in a 5 Si-atoms chain.

Changes in the behavior and magnitude of T as a function of ε on replacing central C-atom by one Si-atom are less drastic in case of 7 C-atoms chain as compared to the case of 5 C-atoms chain, as can be observed from curves in Fig. 2.3(c). This may be because of more number of C atoms on both sides of a Si-atom, which do not allow major change in complex band structure and density of states of 7 C-atoms chain. On replacing one and then two C-atoms in middle of 7 C-atoms chain to form C-C-C-Si-C-C-C and C-C-Si-C-Si-C-C chains, behavior of T versus ε curves change in all three regions A, B and C, as can be seen from Fig. 2.3(c). T values are significantly reduced for -4.0 eV $\leq \varepsilon \leq$ 3.5 eV on replacing central C-atom by Si-atom in 7 C-atoms chain. The energy range is narrowed in C-region and value of

T greatly enhanced in region when two C-atoms are replaced to form C-C-Si-C-Si-C-C atomic chain.

5-atom	Computed $G(E_f)$	7-atom	Computed $G(E_f)$
C-C-C-C-C	0.72627950	C-C-C-C-C-C-C	0.80386785
C-C-Si-C-C	1.465645	C-C-C-Si-C-C-C	0.482197
C-Si-C-Si-C	0.250619	C-C-Si-C-Si-C-C	1.993883
Si- C-Si- C-Si	1.1087415	C-Si- C-Si- C-Si-C	0.1003420
Si- Si- C-Si- Si	1.1553625	Si- C-Si- C-Si-C-Si	0.8332787
Si- Si- Si- Si- Si	2.0041835		
Si-C-C-C-Si	1.8408117		
C-Si-Si-Si-C	1.425634		

Table 1: Values of conductance G at Fermi energy in units of $2e^2/h$ for different chains.

Our computed values of conductance at the Fermi energy, $G(E_f)$ are reported in the table 1 in units of $2e^2/h$ for chains of 5-atoms and 7-atoms. The maximum values of $G(E_f)$ are found for 5 Si-atoms chain (~2.00) and for C-C-Si-C-Si-C-C chain (~1.99). 5 Si-atoms chain yield much higher value of $G(E_f)$ as compared to that for 5 C-atoms chain. In case of 5-atoms chain, minimum value of $G(E_f)$ occurs for C-Si-C-Si-C chain. However, another 5-atoms chain with 3 C-atoms (Si-C-C-C-Si) gives more than 7 time higher value of $G(E_f)$. Similarly both the chains Si-C-Si-C-Si and C-Si-Si-Si-C have 3 Si-atoms and 2 C-atoms. But their $G(E_f)$ are very different. This suggest that positions of C and Si atoms in a chain play important role in determination of $G(E_f)$ as is observed from the table. 5-atoms chain, with Si as end atoms are better conducting as compared to those with C as end atoms.

As can be seen from table, chains of 5 atoms exhibit exactly opposite behavior on increasing Si-atoms as compared to that observed for 7-atom chain. The observed values of $G(E_f)$ for 5 C-atoms and 7 C-atoms chains are not very different from each other. However, when the central C-atom is replaced by Si-atom, $G(E_f)$ for 5-atoms chain increases sharply to the value of 1.465 while for seven-atom chain it decreases to 0.482. Further, when two Si-atoms are included in a chain, $G(E_f)$ for five atom chain reaches to 0.251 while for seven atom chain it goes to 1.994. Again, for 5-atom chain with 3 Si atoms, $G(E_f)$ can go up to 1.42 and for 7-atoms chain it drops to 0.10. On further increasing Si atoms to 4 in a chain, $G(E_f)$ for 5-atoms chain drops to 1.15 while that for 7-atom chain it is enhanced to 0.83. As is observed from the table, 5-atoms chains exhibit higher value of $G(E_f)$ when there are odd number of Si atoms, while for 7-atoms chains $G(E_f)$ is higher for chains that have even number of Si atoms.

Addition of 2 C-atoms at terminal site of Si-C-Si-C-Si chain to make C-Si-C-Si-C-Si-C chain lowers the $G(E_f)$ from 1.10 to 0.10 while adding 2 Si-atoms at terminal site of C-Si-C-Si-C chain to make Si-C-Si-C-Si-C-Si enhances the $G(E_f)$ to 0.83 from 0.25. We find that both 5-atoms and 7-atoms chains with alternate Si-C atoms display significantly enhanced value of $G(E_f)$; roughly 3-10 times higher, when terminal atoms are Si. Our computed conductance results for the chains C-Si-C-Si-C ($G(E_f) = 0.25$), C-Si-C-Si-C-Si-C ($G(E_f) = 0.10$), Si-C-Si-C-Si ($G(E_f) = 1.10$) and Si-C-Si-C-Si-C-Si ($G(E_f) = 0.83$) suggest that chains with alternate Si and C atoms exhibit decreasing $G(E_f)$ on increasing the length of chain. This is in good agreement with the fact that infinite Si-C atomic chain is good insulator.

2.3.2 Si-C atomic chain Attached to Al Bulk

2.3.2.1 Computational Details

In previous section we used 'Al nanorod' as an electrode, which was simulated by introducing vacuum between the periodic images of supercell. This nanorod geometry of Al electrode can be used to have comparative study of atomic chains with different chemistries but do not represent the practical electrode geometries where any probe used to collect current would have hundreds of atoms. As the transport properties of the system also depend on the electrode geometry/size, we tried to find out the difference in transmission coefficient curves when electrodes are simulated to more practical geometry by introducing bulk like nature. Now, electrode supercell does not contain vacuum for separating two periodic images, instead cell-size is managed in such a way that, supercell and its periodic images form a continuous bulk like structure. Si-C atomic chains are sandwiched between these two bulk like electrodes and their electronic transport properties are calculated.

In the previous section we took nanorod as electrodes. In this present section, we consider model contacts made up of a short linear atomic chain of C and Si suspended in vacuum between two semi-infinite ideal Al bulks. The atomic chain made from C and Si is attached at "hollow" sites of two mirror symmetrical Al surfaces. For calculations, a supercell periodicity is employed in the *xy* plane, perpendicular to the nanowire such that there is no vacuum between electrode and its replicas formed in this plane as depicted in the Fig. 2.4.

The spacing between atomic chain and its replica is more than 8 Å which is enough to keep the periodically repeated wires sufficiently apart from one another to make their mutual influence irrelevant. The bulk "leads" are simulated by a planar slab consisting of seven atomic (001) crystalline planes having eight atoms per plane, sufficient to reproduce a bulk-like potential in the middle of the slab. Periodic boundary conditions are assumed in all three

directions for electronic structure calculations. Since the supercell is very large along [001] (the z axis), the BZ is

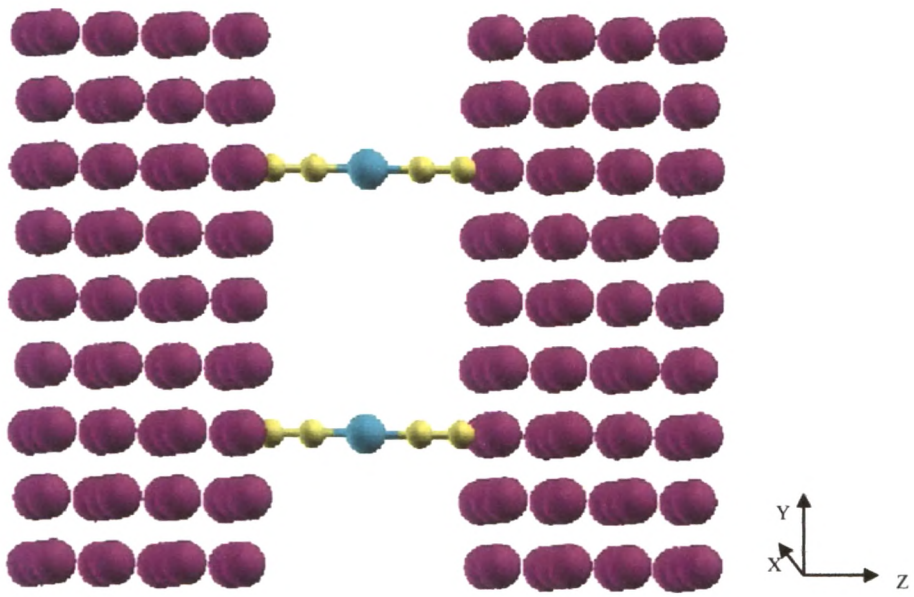

Figure 2.4: A typical electrode-chain-electrode system and its periodic image formed in the y direction. System and its replicas create an effect of bulk electrodes. The distance between two chains is kept more than 8 Å. Similar replicas are formed in x direction also (not shown here). The atomic chain of C (yellow) and Si (blue) is suspended in vacuum between two electrodes.

sampled using special k points generated using Monkhorst-Pack scheme on [4, 4, 2] grid. The energy smearing parameter near E_f was chosen to be 0.01 Ry. Atoms of the seven-layer slab representing the bulk leads are located at their ideal bulk FCC positions, with inter atomic spacing of 2.86 Å. The pseudopotentials and other computational details are same as used in previous section.

2.3.2.2 Results and Discussion

In Figs. 2.5 (a) and (b) display the computed transmission coefficient curves as a function of incident electron energies for 5-atom C-Si chains attached to Al-bulk electrodes. As compared to the case of atomic chains are attached to Al-nanorod electrodes, the striking difference observed is the disappearance of wiggles in the transmission curves. The abrupt changes in transmission curves in Al-nanorod case are smoothened out due to the use of bulk electrodes. This clearly indicates the absence of surface effects which are manifestation of nanorod electrodes. However, we find a qualitative agreement for positions of peaks in transmission curves. Therefore, it can be concluded from these studies that the use of bulk/large electrodes in place of nanorod electrodes could prove better for device making, because of the absence of surface effects.

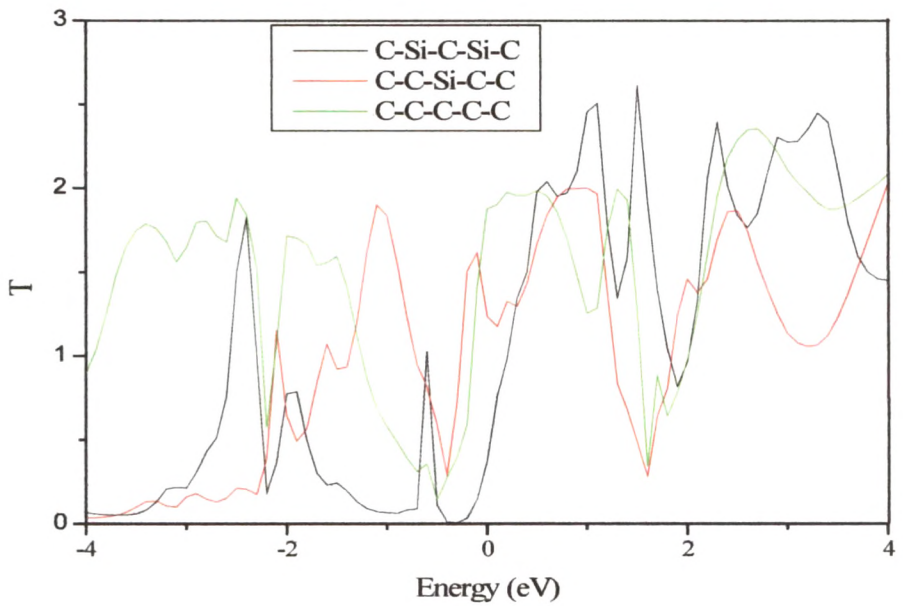

Figure 2.5 (a): Transmission Co-efficient T as a function of ε, energy measured from Fermi level for C-Si-C-Si-C chain, C-C-Si-C-C chain and C-C-C-C-C chain attached to continuous bulk like Al electrodes.

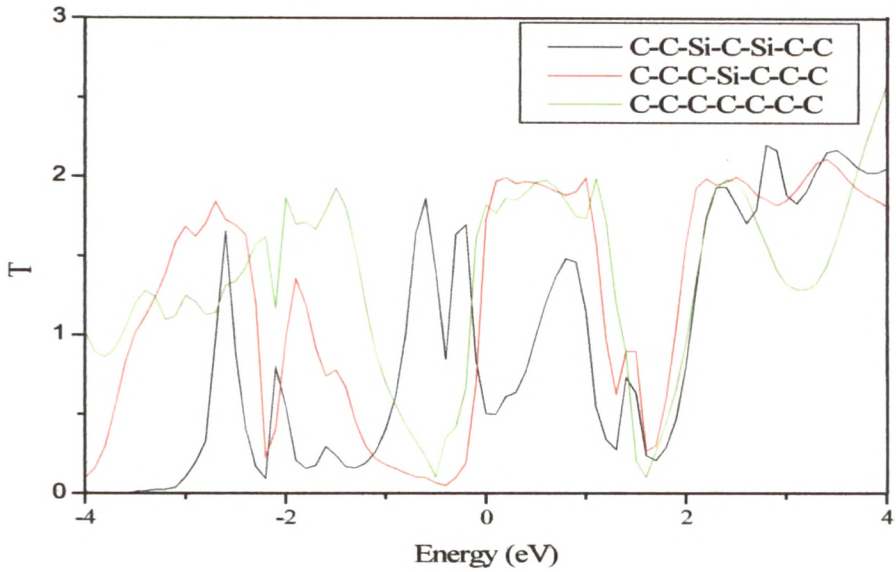

Figure 2.5 (b): Transmission Co-efficient T as a function of ε, energy measured from Fermi level for C-C-Si-C-Si-C-C chain, C-C-C-Si-C-C-C chain and C-C-C-C-C-C-C chain attached to continuous bulk like Al electrodes.

2.3.3 Conclusions

We have studied systems of chains made of C and Si atoms and attached to Al electrodes keeping three main objectives in mind:

i) To check the feasibility of C-Si atomic chains using energetics.

ii) To investigate effects of proposition and positions of C and Si atoms on the transport properties of atomic chains.

iii) To compare the transmission curves obtained in case of Al nanorod and Al bulk electrodes.

Our results on energetics of the C and Si based atomic chain suggest that the synthesis of C-Si chains is practically possible. The computed transmission coefficient is reported for the energy range -4 to 4 eV. Our computed results on T suggest the followings:

1. On varying the number of C and Si atoms, the range of available maximum T changes.
2. The height of peaks, depth of dips, position and width of peaks and dips, and the number of peaks and dips change when relative number of C and Si atoms, total number of atoms and the positions of atoms are changed.
3. Behavior and value of T change and a drastic change in $G(E_f)$ is noted on interchanging the position of C and Si atoms in both the chains of 5-atoms and 7-atoms.
4. Behavior of T versus ε curve and magnitude of $G(E_f)$ very much depend on whether end-atoms in a chain are C-atoms or Si-atoms. The type of the terminal atoms in chain, number of atoms and the positions of atoms influence the structural and electronic properties and eventually the conduction behavior.

Thus, Control of magnitude and behavior of T versus ε curve and $G(E_f)$ is possible by changing total number of atoms, relative number of C and Si atoms and relative positions of C and Si atoms in a chain.

The transmission co-efficient results obtained with the use of Al-bulk electrode provide wiggle free curves and they are found in qualitative agreement with the results obtained for Al nanorod electrode case.

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