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Tuned electronic, optical and mechanical properties of pristine and hetero nanotubes of group IV elements (C, Si and Ge)

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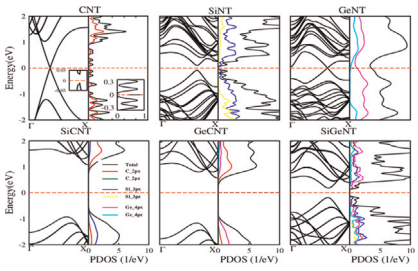
HIGHLIGHTS

- We studied Electronic and Optical properties of Pristine and Hetero Nanotubes.
- The cohesive energy per atom is more for CNT and SiCNT in our study.
- Only GeNT is found to be metallic in nature with a conductance of 2G0.
- Hetero nanotubes have wide band gap spectrum, hence suitable for electronic devices.
- The decreasing order of tensile strength is CNT > SiCNT > GeCNT > SiNT > GeNT > SiGeNT.

GRAPHICAL ABSTRACT

We present electronic band structure of pristine and hetero systems under study.

Electronic band structure and corresponding total and partial DOS for pristine and heteronanotubes. In the inset we have shown the band structure and density of states for CNT in the vicinity of Fermi energy which shows semi-metallic behaviour.



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ABSTRACT

Density functional theory has been used to investigate the structural, electronic, optical and mechanical properties of pristine nanotubes of carbon, silicon, germanium and their hetero nanotubes having armchair conformation with chirality (6,6). In the pristine nanotubes it is found that the cohesive energy per atom is more for CNT as compared to other nanotubes under investigation. However, in hetero systems under study its value is highest for SiCNT system and least for GeCNT. GeNT and SiGeNT have been observed to be more puckered in comparison to other systems. All the pristine and hetero-nanotubes in our study are found to be semiconducting in nature, except GeNT, which is found to be metallic in nature with a conductance of $2G_0$, indicating GeNT to be an ideal material for ballistic transport. Three different types of hetero nanotubes have wide band gap spectrum which opens up an arena for band gap selective engineered devices. The band gap for SiCNT and GeCNT lie in the visible region, while the band gap for other systems lie in the infrared region. The tuning of electronic band structure by means of compression, tensile strain and external electric field indicates that the band gap can be altered considerably. There is a band gap closure under both compression and expansion at a certain value in all the cases except SiCNT, revealing that its band gap can be varied considerably. The decreasing order of tensile strength is CNT > SiCNT > GeCNT > SiNT > GeNT > SiGeNT. The effective mass of holes decreases for pristine systems on the application of compression. Under no strain the effective mass of electrons is generally found to be larger than holes in hetero systems, while it is reverse in

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pristine systems. In case of unstrained systems, we generally observed that the more the effective mass of electron, the more is the band gap in the corresponding system.

1. Introduction

The discovery and the consequent scientific and technological applications of carbon nanotubes have initiated an increasing interest in the field of novel low dimensional materials [1]. Besides carbon nanotubes there are other materials belonging to the same group such as Si and Ge whose nanotubes are also strong contenders for technological applications. Their low dimensionality and the quantum confinement effect can result in fascinating electronic and optical properties [2–5,7,6,8,9]. These nanostructures show potential applications in electronics [3,4], photonics [10], chemical sensors [5], field emission devices [11,7], solar cells [12], electrochemical performances [13], lithium ion battery [14], hydrogen storages [6] and drug delivery [8]. Researchers have put in a lot of efforts to investigate the nanoscale forms of silicon, for miniaturizing the microelectronic devices and to understand new properties that result at the nanoscale [15,16]. In addition to carbon and silicon, germanium (Ge) nanostructure is particularly interesting for future nanotechnology not only because of its similar structural and electronic properties to those of Si but also for many superior properties over Si in device applications [17]. For instance the higher intrinsic carrier mobility of Ge makes it a better channel material for high-performance field-effect logic transistors [18]. The larger excitonic Bohr radius of Ge yields a more pronounced quantum confinement effect than Si [19]. Furthermore, it is a potential anode material in lithium ion batteries, as the diffusivity of lithium in Ge is 400 times faster than in silicon at room temperature [20]. As Ge nanowires and nanotubes based on their properties are well suited as an anode in lithium ion batteries [20,14] compared to thin films, a further option to develop such Ge nanostructures would be of great interest. Germanium nanotubes as long as 2 μm have been grown using template assisted electrodeposition from a room temperature ionic liquid [21]. Preliminary evidence for nanotubecompounds suggests that by virtue of introducing another element, the electronic properties and stability of these tubes can be significantly modified: specifically, band gaps get opened up, as other elements might trap the extra electrons from the tubes [22]. Schmidt and Eberl [23] fabricated SiGe nanotubes experimentally by using the method of the thin-film bending mechanism and found that SiGe nanotubes show excellent mechanical properties, indicating that they could be used as nanodrillers and microscopy tips. The calculations based on density functional theory have reported that SiC nanotubes are semiconducting in nature irrespective of chirality, which is not the case in carbon nanotubes [24,25]. SiC nanotubes are also being successfully synthesized in various laboratories using various methods [26,27] and it has also been suggested that SiC nanotubes can be a potential candidate for hydrogen storage [28]. Rathi and Ray [29] studied the electronic and geometric structures of hydrogenated GeC nanotubes and found the nanotubes to be semiconducting.

Many attempts have been made to explore the ground state geometric and electronic properties of CNTs, SiNTs, GeNTs [30,31,33,32,34–36]. There is a need to systematically study the optical and mechanical properties of these pristine and hetero nanotubes which have only been explored for pristine SiNT [37]. In this study our aim is to compare, the pristine nanotubes of group IV elements (C, Si and Ge) and their heterostructures and their relative stabilities in terms of their characteristic electronic structures. We have looked at the structural, electronic (density of states and band structure), optical and mechanical properties of armchair (6,6) pristine and hetero nanotubes of group IV elements C, Si and Ge. As Compared to other nanotubes, armchair nanotubes have been found to have more stable structures due to the sufficient overlap of p_z orbitals and delocalization of π bonds [38]. Moreover, armchairs with (6,6) chirality have been found to be more stable in comparison to (4,0) and (5,5) configurations [39,40]. Due to this reason we have chosen (6,6) chirality in the present study. For simplicity, the pristine nanotube system is denoted by carbon nanotube (CNT), silicon nanotube (SiNT), germanium nanotube (GeNT) and hetero nanotube systems of silicon–carbon nanotube (SiCNT), germanium–carbon nanotube (GeCNT) and silicon–germanium nanotube (SiGeNT) respectively throughout the paper. The paper is organized as follows: in Section 2, brief computational details are presented. In Section 3, we present the calculated results and discuss these in the light of other available studies. Conclusions are presented in Section 4.

2. Computational details

In our study we have used well tested [37,41,42] Troullier Martin, norm-conserving, relativistic pseudopotentials [43,44] with valence atomic configuration $2s^2 2p^2$, $3s^2 3p^2$ and $4s^2 4p^2$ for C, Si and Ge respectively. The exchange and correlation energies were treated within the generalized gradient approximation (GGA) according to the PBEsol [45] parametrization. Throughout geometry optimization we have used numerical atomic orbitals with double zeta polarization (DZP) basis sets with confinement energy of 20 meV. For Brillouin zone integration, $1 \times 1 \times 30$ Monkhorst-Pack [46] mesh for both pristine and hetero nanotubes has been chosen. The convergence tolerance for the energy was chosen as 10^{-6} eV between two consecutive self-consistent field (SCF) steps. Minimization of the energy was carried out using the standard conjugate-gradients (CG) technique. Structures were relaxed until the forces on each atom were less than 0.01 eV/Å. The mesh cut-off energy used to calculate the Hartree, exchange and correlation contribution to the total energy and Hamiltonian was chosen to be 300 Ry. Also, a vacuum of 30 Å along the *x*-axis and the *y*-axis has been taken to ensure that there is no interaction between neighbouring nanotubes. The fully relaxed structures (*i.e.* minimum energy configuration) for all the systems *viz* CNT, SiNT, GeNT, SiCNT, GeCNT and SiGeNT were obtained by simultaneously relaxing both lattice vectors and atomic positions in unit cell. Pristine nanotubes were modelled by taking 24 atoms per unit cell whereas in the case of heterostructures 12 atoms per corresponding species were taken. In hetero systems the ratio of the corresponding two species is 1:1 at alternate positions.

3. Results and discussions

3.1. Structural properties

Fig. 1 shows a generic tube structure in different views *i.e.* cross-sectional, side and inner views for the systems under study, if atoms are of same type it is pristine and of two types it becomes a heterostructure. Heterogeneity is in the ratio 1:1.