

Energetics and Bandstructure for a Polyacetylene Chain Enclosed inside a Carbon Nanotube

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Abstract

Using density functional theory, we calculate the energy and bandstructure properties of a polyacetylene chain enclosed inside various armchair carbon nanotubes. We find that (4,4) and (5,5) nanotubes are too narrow to contain a polyacetylene chain, while (6,6) nanotubes and wider are energetically favoured to contain one or more polyacetylene chains. Bandstructure calculations reveal that there is some interaction between the enclosed polyacetylene chain and carbon nanotube. Interestingly, we find that this interaction causes a sharp peak to appear in the density of states near the Fermi level, which could facilitate a transition to a superconducting phase.

Keywords: carbon nanotube, polyacetylene, composite

1. Introduction

Carbon nanotubes are hollow cylindrical structures which could make ideal containers for just a few atoms or small molecules. In this regard, they have been considered for hydrogen storage [1] and as nano-sized ‘test-tubes for manipulating chemical/biological molecules’ [2]. If one is interested in investigating one-dimensional nano-systems then carbon nanotubes could act as a support structure to contain the nano-system. For example, nanotubes have been considered for confining a one-dimensional chain of metal atoms [3], where the interest lies in comparing the properties of the one-dimensional chain with that of the bulk three-dimensional metal.

Another one-dimensional material of considerable interest is polyacetylene (PA). Unlike metallic carbon nanotubes [4], polyacetylene succumbs to Peierls distortion so that pure PA has a dimerized structure with a bandgap opened up at the Fermi level. In lightly doped PA the charge carriers are the somewhat more exotic solitons which can carry spin and no charge or charge and no spin [5]. Highly doped polyacetylene is a good metal so, like carbon nanotubes, potentially has widescale technological applications.

In bulk PA the intrinsic properties of the PA chains may be obscured due to inter-chain coupling, complicated morphology of the bulk material or effects coming from dopant atoms. To avoid these sources of disorder, it would be desirable to isolate out a single PA chain for investigation. In order to keep the PA chain straight, so that

defects from chain bending do not arise, we suggest that a carbon nanotube could act as a support structure to restrain the PA chain. Hence, in this paper we theoretically investigate properties of a PA chain contained inside a carbon nanotube.

2. Method of Calculation

Calculations were performed with density functional theory (DFT) under the local density approximation (LDA) using SIESTA [6]. In all cases, the axes of the PA chain and carbon nanotube were kept parallel. To reduce computing requirements, only armchair nanotubes were considered. Since the lattice structure of a PA chain and graphitic armchair nanotube are very similar, this allowed the PA lattice to be held commensurate with the nanotube lattice, thus reducing the number of atoms required per unit cell. Depending on the size of the carbon nanotube being considered, the unit cell contained between 20 atoms (for a (4,4) nanotube) and 32 atoms (for a (7,7) nanotube). Of these, two carbon atoms and two hydrogen atoms were associated with the PA chain. The unit cell size perpendicular to the carbon nanotube axis was set to at least 10 Angstroms so that there was no interaction between structures in adjacent cells

3. Results

Figure 1 shows our result for a PA chain inside armchair carbon nanotubes of various radii. For a (4,4) nanotube (not

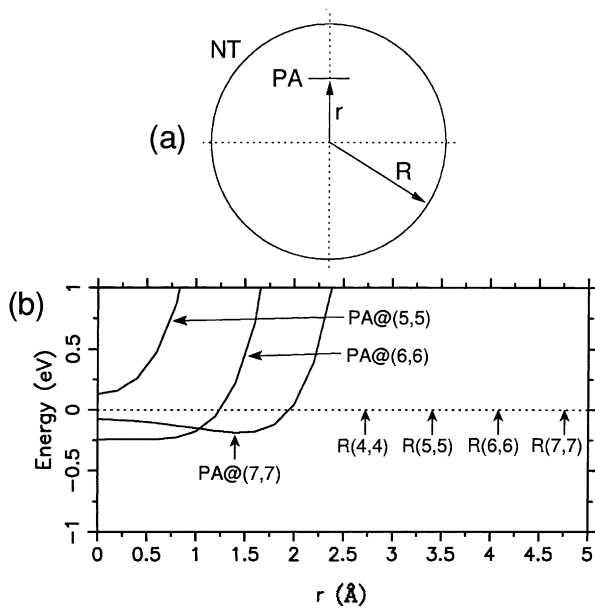


Fig. 1. (a) Schematic diagram illustrating the r -axis for the results in (b). (b) Interaction energy between various (n,n) nanotubes and an enclosed PA chain. Vertical arrows for R(4,4), R(5,5), R(6,6) and R(7,7) indicate the wall of (4,4), (5,5), (6,6) and (7,7) nanotubes respectively.

shown) the interaction energy is $E > 4$ eV for all r , indicating that this configuration is highly energetically unfavourable. Also for the (5,5) nanotube, the interaction energy remains positive for all r so that this configuration is energetically unfavourable, although, just marginally so. For the (6,6) and (7,7) nanotubes, the nanotube diameter is sufficient to allow a negative energy minimum to appear inside the nanotube. Hence, these configurations are energetically favourable. For the (6,6) nanotube, the minimum is fairly wide so that a PA chain enclosed inside a (6,6) nanotube would still have some degree of lateral freedom. The (7,7) nanotube is sufficiently wide for two energy minima to appear inside the nanotube such that two PA chains could be accommodated.

Figure 2 shows the bandstructure for a PA chain inside a (7,7) nanotube. We find that the bandstructure for the combined system is not an algebraic sum of the separate PA and nanotube bandstructures. This highlights that there is some interaction between the PA chain and nanotube. Of interest is that one of the DOS peaks originating from the PA chain coincides with the Fermi level. If the nanotube/PA system is susceptible to a superconducting phase transition [7] then such a peak in the DOS at the Fermi level could enhance the superconducting transition temperature [8]. This can be seen from the weak coupled BCS theory where the transition temperature is given by $T_c \sim \hbar\omega_D \exp(-1/\lambda)$ with $\lambda = N(E_f) V_0$. $N(E_f)$ is the DOS at the Fermi level and V_0 is due to the electron-phonon interaction. An increase in $N(E_f)$ due to a peak in the DOS at the Fermi level would increase T_c .

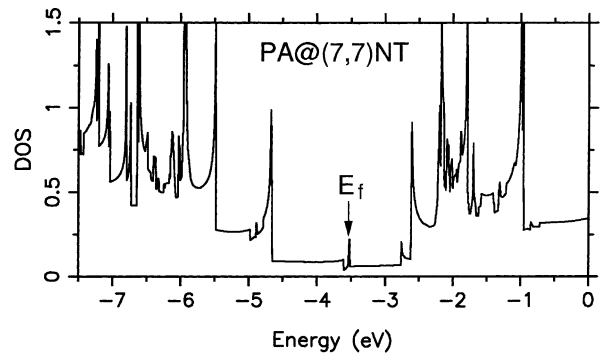


Fig. 2. DOS for a PA chain inside a (7,7) nanotube.

4. Summary

We have investigated the possibility of containing a PA chain inside an armchair carbon nanotube. We find a (4,4) or (5,5) nanotube is too narrow while a (6,6) nanotube could contain a single PA chain, albeit, with some lateral freedom. On the other hand, a larger nanotube such as the (10,10) nanotube could contain 2 or more PA chains.

Bandstructure calculations reveal that there is some interaction between the enclosed PA chain and carbon nanotube so that using the carbon nanotube as an inert shield for the PA chain may not be achievable. In this regard, an investigation of boron-nitride nanotubes would be worthwhile [3]. Of interest is the finding that the bandstructure calculation for the combined system yields a peak in the DOS near the Fermi level which could facilitate a transition to a collective phase such as superconductivity.

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