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Electronic transport in single-helical protein molecules: Effects of multiple charge conduction pathways and helical symmetry

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ABSTRACT

We propose a tight-binding model to investigate electronic transport properties of single helical protein molecules incorporating both the helical symmetry and the possibility of multiple charge transfer pathways. Our study reveals that due to existence of both the multiple charge transfer pathways and helical symmetry, the transport properties are quite rigid under influence of environmental fluctuations which indicates that these biomolecules can serve as better alternatives in nanoelectronic devices than its other biological counterparts *e.g.*, single-stranded DNA.

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1. Introduction

Current days biomolecules are receiving huge attention from different scientific communities including physics, chemistry and others because of their possible applications in nanoelectronics and the need of understanding electronic and spin transfer processes in biological systems [1–4]. DNA is one of them which has attracted major attention from the beginning of the last decade [5–9]. Whereas other biomolecules such as proteins are less attended in this respect. However with the recent progress in chiral-induced spin selectivity (CISS) both DNA and protein are getting similar attraction [10–22] across various disciplines as they both have helical structures which can be used for efficient spin polarization. In 2011 Göhler et al. [10] showed that double-stranded DNA (ds-DNA) can be used as a good spin filtering agent with length dependent spin polarization up to 60%. Whereas no spin polarization was achieved for single-stranded DNA (ss-DNA). These findings are then theoretically supported by Guo et al. [12]. But recent experiments suggest that α-helical proteins are also quite efficient in spin polarization process though it has single helical structure [21,22]. These results open up an opportunity to examine these single-helical structures from a new aspect, different models are also proposed to explain these experimental results [14]. In respect of electronic transport properties DNA is widely studied, though there are still controversies over different experimental results [7–9,23–26]. Questions still remain on reproducibility of the experimental data and underlying charge transfer mechanism [27,29,28,30–33]. Whereas the same properties of different protein molecules are less examined. There are only a few reports available in the literature on electronic transfer process in proteins [34–38], but no such report is available on the effects of environment on its electronic transport properties. It is confirmed by CISS study and related theoretical work that there are multiple charge conduction pathways (MCCP) present in single-helical proteins due to which they are able to polarize the electron spin [14,21,22]. This possibility of MCCP makes helical protein molecules very good agents for long-range charge transport. As proteins have these MCCP, electrons will face less disturbances/environmental effects during conduction and transport characteristics will be much rigid; reproduction of the experimental results will be much simpler with them.

In this paper we make an attempt to study the electronic transport properties of single helical proteins incorporating both the helical symmetry and possibility of MCCP within tight-binding framework. We propose a model Hamiltonian to explore electronic transport through single-helical proteins and compare our results with another model proposed in Ref. [14]. We study different transport properties from localization behavior to I–V response including the effects of environment that are modeled in terms of disordered on-site potential of the amino acids within the tight-binding Hamiltonian. Our investigations show that due to presence of MCCP the effects of environment are much smaller which enable long range coherent charge transfer in these biomolecules. Interplay of helical symmetry and disorder also has non-trivial effects on localization and I–V responses of the protein molecules.

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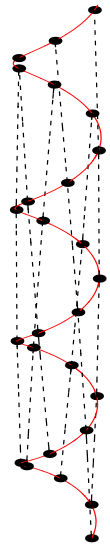

Fig. 1. (Color online.) Schematic diagram of a single-helical protein molecule. Black dots on the helix represent the amino acids and dotted (black) lines between those black dots represent hopping (t') between neighboring amino acids of adjacent pitches. The red line shows the single helix.

2. Theoretical formulation

The two-terminal electronic transport through single-helical protein molecule can be simulated using the following tight-binding Hamiltonian for the entire system

$$H_{tot} = H_{pro} + H_{leads} + H_{tun} \,, \tag{1}$$

where H_{pro} is the Hamiltonian for the protein molecule, H_{leads} represents the one dimensional semi-infinite leads on the both sides of the protein molecule and H_{tun} is the tunneling Hamiltonian between protein molecule and the leads. The tight-binding Hamiltonian (Fig. 1) for the protein molecule is formed on the basis set spanned by the amino acids

$$H_{pro} = \sum_{i=1}^{N} \epsilon c_i^\dagger c_i + \sum_{i=1}^{N-1} t c_i^\dagger c_{i+1} + \sum_{i=1}^{N-n} t' c_i^\dagger c_{i+n} + \text{H.c.} \,, \tag{2}$$

where $c_i^\dagger$ (c_i) is the creation (annihilation) operator for electrons at the ith Wannier state of the protein molecule with length N, $t =$ nearest neighbor hopping amplitude, $\epsilon =$ on-site potential energy of the amino acids, $t' =$ hopping integral between two neighboring atomic sites in adjacent pitches which incorporates the possibility of MCCP along the helix. Here n is the number of amino acids within a given pitch, parameter that accounts for the helical symmetry. A dispersion relation for an infinite homogeneous chain of protein molecule can be obtained following the above Hamiltonian: $E = \epsilon + 2t\cos(k) + 2t'\cos(nk)$ which explicitly depends on helical symmetry (n).

Apart from the above model, we also use another model following Ref. [14] to compare our results. The protein molecule is described in this model following the tight-binding Hamiltonian (later on we refer this as model:2 throughout the paper)

$$H_{pro} = \sum_{i=1}^{N} \epsilon c_i^\dagger c_i + \sum_{i=1}^{N-1} \sum_{j=1}^{N-i} t_j c_i^\dagger c_{i+j} + \text{H.c.} \,, \tag{3}$$

where $c_i^\dagger$, c_i, ϵ and N have their usual meanings. $t_j = t_1 e^{-(l_j - l_1)/l_c}$ is the jth neighboring hopping amplitude, where l_j is the distance between two neighbors i and $i+j$, l_c is the decay exponent and t_1 is the nearest neighbor hopping integral. Here we have assumed that the electronic wave functions decay exponentially over distance. These assumptions are similar to the Slater–Koster scheme, and l_c can be obtained by matching to first-principle calculations [1,14].

In order to study the transport behavior of protein molecules, we use semi-infinite 1D chains as leads connected to the left (L) and right (R) ends of the protein molecule and the corresponding Hamiltonian can be expressed as

$$H_{leads} = \sum_i \left(\epsilon c_i^\dagger c_i + t c_i^\dagger c_{i+1} + \text{H.c.} \right) \,, \tag{4}$$

where $i < 0$ and $i > N$ respectively represent left and right semi-infinite 1D leads. The tunneling Hamiltonian between the leads and protein molecule is given by $H_{tun} = \tau \left(c_0^\dagger c_1 + c_N^\dagger c_{N+1} + \text{H.c.} \right)$ where τ is the tunneling matrix element between protein and the leads. In order to obtain transmission probability $T(E)$ of electron through single-helical protein we use the Green's function formalism [39]. The single particle retarded Green's function for the entire system at an energy E is given by $G^r = (E - H + i\eta)^{-1}$, where $\eta \to 0^+$. The transmission probability of an electron with incident energy E is given by $T(E) = \text{Tr}[\Gamma_L G^r \Gamma_R G^a]$ where Tr represents trace over reduced Hilbert space spanned by the protein molecule. The retarded and the advanced Green's functions in the reduced Hilbert space can be expressed as $G^r = [G^a]^\dagger = [E - H_{pro} - \Sigma_L^r - \Sigma_R^r + i\eta]^{-1}$, where $\Sigma_{L(R)}^{r(a)} = H_{tun}^\dagger G_{L(R)}^{r(a)} H_{tun}$ is retarded (advanced) self-energy of the left (right) lead and $\Gamma_{L(R)} = i[\Sigma_{L(R)}^r - \Sigma_{L(R)}^a]$ is the level broadening due to coupling of the leads with the protein molecule, $G_{L(R)}^{r(a)}$ being the retarded (advanced) Green's function for the left (right) lead. It can easily be shown that $\Gamma_{L(R)} = -2\ \text{Im}(\Sigma_{L(R)}^r)$, where Im represents the imaginary part. At absolute zero temperature, using the Landauer formula, current through the protein molecule for an applied bias voltage V is given by $I(V) = \frac{2e}{h} \int_{E_F - eV/2}^{E_F + eV/2} T(E) dE$, where E_F is the Fermi energy. We have assumed that voltage drop occurs only at the boundaries of the conductor.

3. Results

To perform numerical calculations we use following parameter values for our proposed model throughout the entire work: $\epsilon = 0$ eV, $t = 1.0$ eV and $t' = t/10 = 0.1$ eV. We compare our results with model:2 using the following parameters: $l_1 = 4.1$, $l_2 = 5.8$, $l_3 = 5.1$, $l_4 = 6.2$, $l_5 = 8.9$, $l_6 = 10.0$ and l_c is taken as 0.9, all units are in Å. Using these values we can calculate the related hopping integrals (t_j) which gives $t_2 \sim 0.16 t_1$ and so on. It is clear that gradually t_j values will decrease (except $t_3 > t_2$) with increasing distance, therefore we restrict ourselves to t_6 and set $t_1 = t = 1.0$ eV. These parameter values for model:2 are extracted from Ref. [14]. For ss-DNA, to calculate its transport properties, we set $t' = 0$ eV in our model which cancels any possibility of MCCP. We first study the localization properties of the system. The localization length (l) of the system is calculated from the Lyapunov exponent (γ) [40]

$$\gamma = 1/l = -\lim_{N \to \infty} \frac{1}{2N} < \ln(T(E)) > \,, \tag{5}$$

where $N =$ length of the system and $<>$ denotes average over different disorder configurations. In actual experiments there are various environmental fluctuations that we have simulated in the model by considering the on-site energy of the amino acids (ϵ) to be randomly distributed within the range $[\epsilon - \text{w}/2, \epsilon + \text{w}/2]$, where w represents the disorder strength.

In Fig. 2 we show the variation of Lyapunov exponent with disorder at different energies for both the protein molecule and

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