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Electronic transport on the spatial structure of the protein: Three-dimensional lattice model

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ABSTRACT

We report a numerical analysis of the electronic transport in protein chain consisting of thirty-six standard amino acids. The protein chains studied have three-dimensional structure, which can present itself in three distinct conformations and the difference consist in the presence or absence of thirteen hydrogen-bondings. Our theoretical method uses an electronic tight-binding Hamiltonian model, appropriate to describe the protein segments modeled by the amino acid chain. We note that the presence and the permutations between weak bonds in the structure of proteins are directly related to the signing of the current–voltage. Furthermore, the electronic transport depends on the effect of temperature. In addition, we have found a semiconductor behave in the models investigated and it suggest a potential application in the development of novel biosensors for molecular diagnostics.

1. Introduction

Proteins are the main functional elements in all living organisms. In biological systems, the genetic information stored in DNA is transcribed by the mRNA. The combinations of three of the four nucleotides of the mRNA identify an amino acid, known as tRNA, which assists in the translation of the genetic code contained in DNA and mRNA, thereby producing a specific protein [1,2]. Therefore, proteins are macromolecules consisting of a chain of amino acid residues linked by peptide bonds, thus forming a primary structure.

The biological function of a protein is related to its spatial structure, in other words the primary structure has to bend to form a secondary structure and then packaged in a tertiary structure. In some cases, the tertiary structures of several proteins or subunits have joined to form the quaternary structure. That last structure is kept stable by several weak bonds among the subunits of the same kind, which maintain the tertiary structure. Some agents may cause changing in the protein conformation, such as: temperature, changing in the medium acidity, and substitution of a single amino acid [2,3]. Following the twenty standard amino acids which form all proteins are represented in Table 1. The spatial organization of the protein depends on the amino acid comprising and as they are available in relation to others in the chain. [2,3].

Table 1
The twenty standard amino acids.

Alanine (A)	Cysteine (C)	Aspartic Acid (D)	Glutamic Acid (E)
Phenylalanine (F)	Glycine (G)	Histidine (H)	Isoleucine (I)
Lysine (K)	Leucine (L)	Methionine (M)	Asparagine (N)
Proline (P)	Glutamine (Q)	Arginine (R)	Serine (S)
Threonine (T)	Valine (V)	Tryptophan (W)	Tyrosine (Y)

Nowadays, biomolecules are strong candidates to be part of sensors for diagnosis and prognosis in biomedical area. Generally, enzymes (proteins) are often used in sensors due to their specificity and the reaction products may be electrochemical transducer for measurement. When enzymes are immobilized by an electrode enzymatic reactions is activated and can be translated by electron transport [4,5].

The idea of using biomolecules as electronic components is not new. In 1974, Aviram and Ratner were the ones who first suggested the construction of a simple organic electronic device, called a rectifier, which is composed of a donor and an acceptor system connected by a bridge of carbon single bonds [6]. Since then, the charge transport through an electrode–molecule–electrode junction is extensively studied and it is of key importance in molecular electronics applications [7–10].

The aim of this study is to investigate the electronic transport in a three dimensional lattice model, which is represented in three

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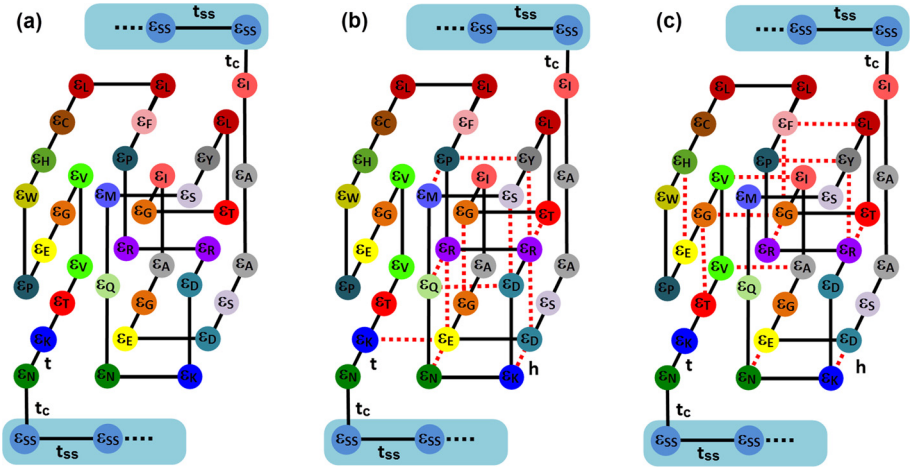

Fig. 1. Schematic models for the electron transport in three types of proteins represented in three dimensional structure, where (a) P_A, (b) P_B, and (c) P_C connected between two electrodes. The circles denote sites (electrode or amino acid); the solid lines represent the peptide bonds ($t_c = 0.3$ eV is the hopping term between electrode and chain and $t = 0.3$ eV is a peptide bonds energy); the dashed lines denote several hopping terms ($h = 0.03$ eV, hydrogen bonds).

different conformations labeled as P_A, P_B, and P_C. These models have a specific amino acid sequence, differing each other by the hydrogen bondings distribution (see Fig. 1), where thirteen hydrogen bonds try to mimic a mutation (disease) in a real protein as suggested by [11]. For the three proteins under consideration, we take into account the chains of proteins made up of thirty-six amino acids obeying the following sequence NKTVVGEPWHCLLFPRRDKNQMSYLTGIAGEDSAAI. The protein P_A has a simple structural arrangement built of amino acids linked by covalent bonds (peptide bonds). The proteins P_A and P_B present a structural arrangement created of amino acids joined through peptide bonds and non-covalent bonds (hydrogen bonds). We carried out the electronic transport analysis of the protein by fixing the protein between two electrodes. When a potential difference is applied across it, we can obtain an electronic signature of the protein on the effects of low temperature and its protein conformation, serving as a parameter for possible disease investigations or for future applications in nanotechnology.

2. Model and implementation

To address the influence of the previously mentioned factors on the charge transport efficiency, we used the time independent Schrodinger equation to calculate the current–voltage for spatial structure of the protein. The tight-binding model Hamiltonian that describes the electronic transport, through electrode–protein–electrode system, is given by (see Fig. 1):

$$H = H_p + H_e + H_c. \tag{1}$$

The first term on the right side of Eq. (1) describes the hamiltonian through the protein chain and it can be written as

$$H_p = \sum_{i=1}^{36} \varepsilon_i |i\rangle\langle i| + \sum_{i=1}^{35} \left[t_{i,i\pm1} cos(\theta) |i\rangle\langle i \pm 1| \right] + \sum_{i\neq j}^{13} \left[h_{i,j} cos(\theta) |i\rangle\langle j| \right], \tag{2}$$

where $|i\rangle$ represents a localized state of an electron at the i-th amino acid. The quantities $t_{i,i+1}$ and $h_{i,j}$ are the nearest-neighbor electronic overlaps (hopping terms) between the amino acid in protein chain, with their values respectively given by 0.3 eV and 0.03 eV. Each one values are within the range of values obtained by Chemical Quantum Calculation [12]. The term $t_{i,i+1}$ represents the peptide bond energy and $h_{i,j}$ represents hydrogen bond energy, that are weak intermolecular bonds in comparison to peptide bonds, depicted in Figs. 1(b) and 1(c) by t (solid line) and h (dashed line). Despite the hydrogen bonds $h_{i,j}$ to be weak, the large quantities and the form how the bonds are arranged among amino acids, in the chain, can stabilize and to determine the spatial structure of the proteins. Here, we consider 13 connections useful to stabilize these conformational arrangements as it is possible to be seen in Table 2.

Table 2
Connections among amino acid residues. The indexes i and j identify the amino acids at sequence previously cited and numbered from 1 to 36.

Protein P_B				Protein P_C			
i	j	i	j	i	j	i	j
2	31	17	32	3	6	15	24
15	22	18	21	4	29	16	27
15	24	18	23	5	23	17	24
16	21	19	32	6	27	17	26
16	31	20	31	7	10	19	32
17	24	27	30	14	25	20	31
17	26			14	27		

Table 3
The average values of the ionization energy of each specific amino acid $A, B, ..., Y$.

$\varepsilon_A = 8.84$ eV	$\varepsilon_C = 8.68$ eV	$\varepsilon_D = 8.34$ eV	$\varepsilon_E = 7.99$ eV
$\varepsilon_F = 9.24$ eV	$\varepsilon_G = 8.00$ eV	$\varepsilon_H = 8.72$ eV	$\varepsilon_I = 8.77$ eV
$\varepsilon_K = 8.15$ eV	$\varepsilon_L = 8.88$ eV	$\varepsilon_M = 8.41$ eV	$\varepsilon_N = 8.51$ eV
$\varepsilon_P = 8.75$ eV	$\varepsilon_Q = 8.35$ eV	$\varepsilon_R = 8.17$ eV	$\varepsilon_S = 8.34$ eV
$\varepsilon_T = 8.54$ eV	$\varepsilon_V = 8.51$ eV	$\varepsilon_W = 8.32$ eV	$\varepsilon_Y = 8.87$ eV

In Table 3, the variable ε_i represents the energy on-site matrix elements, which is given by the average values of the energy of ionization of the nucleic acids of RNA, i.e., $\varepsilon_G = 7.77$ eV (Guanine), $\varepsilon_C = 8.68$ eV (Cytosine), $\varepsilon_A = 8.26$ eV (Adenine) and $\varepsilon_U = 9.32$ eV (Uracil); that was estimated by V. M. Orlov and collaborators, using photoionization mass-spectrometry in gas phase [13–15].

To investigate the electron transport behavior in a spatial structure of the protein on the effects of temperature, which is known to be one of the principal parameters in experiments with biomolecules, since variation of the temperature induces structural disorder and fluctuations of the system. Thus, we consider the variation of the temperature to the hopping integrals in terms of twist-angle fluctuations. In this context, we assume θ being the twist-angle fluctuations between neighboring amino acid, which means the angle of torsion applied along a chemi-

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