Electric field-dependent charge transport in a poly (dA)-(dT) DNA molecule: localization length study

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Abstract. Electronic transport in DNA molecules could depend on many factors, one of them is external electric field influence. In this research we analyse localization length of poly (dA)-(dT) DNA molecule to study its electron transport properties. Tight binding Hamiltonian model is used along with electric field and temperature influence. Electric field is set to be parallel to the helix axis of DNA. Transfer-matrix method is required to calculate localization length, while gram-schmidt orthonormalization method is used to reduce errors. The results show that electric field changes localization length in all energy considered in calculation.

1. Introduction
In many decades researcher is constantly trying to make smaller and more advance electronics circuits. Silicon based microprocessors has been widely used in today electronics industry, but trial in shrinking the size of it has been started to reach its limits. This challenges scientist to find another alternative materials to be the next generation of nano-device. In 1962 it was proposed that evidently DNA can conduct electrical current [1], this outcome may have inspired scientist to create biomolecular nano-device based on DNA molecule. The process of electron transport is believed because of the π-π stacking interactions along the base pairs and also the phosphate backbone sugar molecules [2]. Charge hopping mechanism is used to describe long range electron transport in DNA where it also occurs between hydrogen bonds in either Guanine-Cytocine or Adenine-Thymine [3].

There are many discoveries regarding DNA conductivity, and some of experimental results indicate the behavior of DNA as insulator [4] and even its behavior as superconductor [5]. This variation in result could happens because DNA is very sensitive to changes due to factors, such as electric field [6], magnetic field [7], temperature [8], and base motion [9] that will alter its structure. Alteration on DNA structure could mainly determine its quality for charge transport. This research will be discussed external electric field influence on electron localization length in poly(dA)-(dT) DNA molecule. In our calculation tight binding hamiltonian model is used to describe interaction between each base and backbone molecule, with adding electric field and temperature contribution. Electric field is set to be parallel to the helix axis of DNA. Transfer-matrix method is also required to calculate localization length, while gram-schmidt orthonormalization method is used to reduce errors. Miller-Abraham formula is used to modify hopping contant that had been affected by electric field. We also consider electron hopping between backbone in our calculation. The results will be represented in terms of localization length that will be elaborated in third section. Finally, the paper will be concluded in the final section.

2. Theoretical model
Double strand DNA molecule, which consist one strand of Adenine (A) base sequence and Thymine (T) base sequence as its complement, is used as medium for electron to transfer. Both ends of DNA strands are attached to electrode molecules which give different potential in between. In this calculation, we assume that electron could travel from base to nearest bases within the same strand, its
pair, and also nearest backbone or vice versa. Along with that, electron also could travel from backbone to nearest backbone. A schematic diagram of a DNA model can be found in the reference [10], and the tight binding Hamiltonian model is determined by: [10]

\[ H = \sum_{i=1}^{N} \sum_{\tau, \sigma=1}^{4} (\varepsilon_{i}^{\tau} + \phi_{i}^{\tau}) |i, \tau, \sigma| + t_{ij}^{\tau,\sigma} |i, \tau, \sigma|^{\dagger} |i+1, \sigma| + \text{h.c} \] (1)

Symbol \( N, i \), and \( \tau (\sigma) \) in equation (1), consecutively, are the length of the molecule sequence (102 base pairs), site index, strand index. Parameter \( \varepsilon_{i}^{\tau} \) is on-site energy of base (9.06 eV for T and 8.22 eV for A), while \( \phi_{i}^{\tau} \) is phonon effect on DNA base on-site energy. Parameter \( t_{ij}^{\tau,\sigma} \) represents electron hopping constant between sites. Medium and temperature are considered to be able to make backbone on-site energy randomly distributed around 9.36 eV with a deviation of 0.1 eV. External electric field is set to be parallel to the helix axis of DNA (z-axis). When we give electric field to the system, it will change electron hopping constant from site \( i \) to \( j \) that is described by the following formula [11],

\[ t_{ij} = t_{0} \exp \left( \frac{qV}{k_{B}T} \cos \theta \right) Z_{ij} - \left( \frac{e^{\tau} - \varepsilon_{i}}{k_{B}T} \right) \] (2)

where \( Z_{ij} \) is the distance between site \( i \) to \( j \), \( q \) is electron charge, \( \theta \) is the angle between \( Z_{ij} \) and electric field, and \( k_{B}T \) is energy unit. \( V \) is voltage difference across the molecule, higher voltages mean higher electric field.

Localization length is giving information to what extent electrons could travel in DNA molecule. By analyzing localization length we could choose which DNA model and sequence is better to be molecular wire. The localization length is calculated by employing transfer matrix method. Due to large number of matrices multiplication, Gram-schmidt orthonormalization method is used to reduce errors. This method will produce coefficient value that is used to calculate Lyapunov exponents using equation:

\[ \delta_{cl} = \frac{\langle \log |P_{cl} | \rangle}{2R(N-1)} \] (3)

where \( cl \) is sequence of matrix columns, \( \beta \) is normalization coefficient, \( R \) is repetition of multiplication, \( N \) is the length of DNA and \( m \) is orthonormalization number. Smallest value of \( \delta \) is used in obtaining localization length \( (\lambda) \) through relation [12]

\[ \lambda = \frac{1}{\delta} \] (4)

3. Results and discussion

The results of the calculation are showed in figure 1 and figure 2. Figure 1 shows electron localization length in DNA poly(dA)-(dT) calculated at temperature 4.2 K. In the spectrum, it appears three regions of energy where the localization length larger than zero, they are around the energy of 7.5 eV – 8 eV (band I); 8.75 eV – 9.25 eV (band II); and 9.5 eV – 9.9 eV (band III). Electronic state in band I are localized states where the value of localization length less than \( N \) (102 pairs). According to Suhendro et al, localized states occurs because of disorder in backbone onsite energy along with thermal agitation caused disorder in effective bases onsite energy, however the difference between backbone onsite energy and bases onsite energy in few electronic energy states are quite small to obtain extended states [13]. Band II and III show some extended states, a condition when the value of localization length more than \( N \). In extended states, the mobility of electron is higher than in localized states, it means that electron can transfer from first base pair to the next 102 pairs. This circumstance in quantum mechanics occurs due to the wavefunction of electron in one quantum state significantly overlap with the neighboring quantum states.

Electric field applied parallel to the helix axis of the poly(dA)-(dT) DNA could change energy states which accordingly change its localization length. It can be seen from figure 1, as we set the value of electric field higher (0.005–5 V), the localization length is decreasing. The width of energy gap also seems increasing, especially in high electric field (5 V), whereas the extended states region looks narrowed. It could be translated that charge transport in DNA poly(dA)-(dT) will be compromised by the presence of electric field. This phenomenon occurs because, in our model, electric field changes the electron hopping constant such that it decreases when electron moves in the direction of electric field and it is constant otherwise.
Figure 1. Localization length of poly(dA)-poly(dT) DNA in various voltage at 4.2 K

Figure 2 shows electron localization length calculated at higher temperature, 30 K. We still observed three energy region with localization length larger than zero separated by two gap with zero localization length. It appears that the localization length decreases significantly with the temperature, thus all three energy region become localized. Higher temperature will affect standard deviation of twist angle distribution to become wider. In consequence, it would causes variation in intrastrand and interstrand hopping amplitudes among bases, and induce onsite energy disorder that block charge transport process in the DNA molecule [14]. Thermal energy changes the onsite energy of bases which produces negative impact on energy structure of DNA molecule. The energy structure of DNA molecule becomes more disorder as the temperature increases. Since we set small magnitude of twisting motion frequency (0.51 meV), the system is furthermore disordered. The results show that thermal fluctuation causes bigger changes in the localization length than the electric field. The same tendency as in figure 1 in which terms of localization length decrement due to voltage increment is observed, but the voltage increase could only slightly change the localization length.
4. Conclusions
The electric field influence of electron localization length in a poly(dA)-(dT) DNA molecule have been studied. The localization length had been calculated by using transfer matrix method. Miller-Abraham formula is used to modify hopping constant under influence of electric field. The results show that higher electric field results in lower localization length in some energy. Higher electric result in wider gap between two energy regions (energy band) with nonzero localization, in consequences the energy band appears narrower. Under the model used in this study, at higher voltage the poly(dA)-(dT) DNA molecule would be less conductive. This tendency is observed in both temperature used in the study. In addition, higher temperature also decreases the mobility of electron to transfer.

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