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MAGNETIC FIELD-DEPENDENT ELECTRIC CURRENT ON A PERIODIC POLY(DA)-POLY(DT) DNA MOLECULE STRUCTURE

Efta Yudiarsah*

Departemen Fisika, FMIPA, Universitas Indonesia, Depok, Jawa Barat, Indonesia

*Corresponding Author Email: e.yudiarsah@sci.ui.ac.id

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ABSTRACT

An electric current flowing on the Poly(dA)-poly(dT) DNA molecule structure has been calculated. The current was calculated from transmission probabilities by employing Landauer-Buttiker formalism. Green's function technique has been used for obtaining the transmission probabilities. The DNA molecule structure was modeled within the tight-binding Hamiltonian model approach. The model takes into account electron hopping parameters which are dependent on the magnetic field as well as the electric field. The presence of a magnetic field causes the Peierls phase factor on the electron hopping parameters. The calculation results at low electric voltages show that after decreasing, the electric current oscillates with the magnetic field. However, at higher electric voltages, the electric current is increasing and oscillates with the magnetic field.

Keywords: electric current, DNA molecule, Poly(dA)-poly(dT), magnetic field

INTRODUCTION

In 1962, Eley and Spivey reported that DNA molecules can conduct electric current [1]. The report enhanced the researcher's interest in this molecule. Several research groups investigate the possibility of using a DNA molecule as an active element in electronic devices for nanotechnology applications such as biosensors [2], molecular size wires [3,4], molecular-based transistors, and other devices [5]. Not only research on the application of DNA molecules but at the same time several groups experimentally as well as theoretically investigated the electron transport mechanism in a DNA molecule under various conditions [6-8]. The I-V characteristic measurements show that a periodic double-strand DNA molecule, poly(dG)-poly(dC), behaves as a semiconductor [3] and also a conductor [9]. However, experiments on an aperiodic DNA molecule show the I-V characteristic of a superconductor material if the measurement is done at low temperatures [10] and isolator [11].

To explain the measurement results which seem to be contradictive, various factors have been considered in the theoretical study. The factors considered to have an essential role in electron transport are, among others, the Watson-Crick base pair sequence of DNA molecule [12-15], the presence of base pair mismatch [16] and void, and environmental effects such as medium and substrate [7,15] as well as temperature [17]. DNA molecule is a soft molecule such that a thermal agitation can make the DNA base vibrate [13,18]. In addition**,** the presence of a magnetic field [19, 20] and electric field as well as molecule-electrode interaction [21] have been considered in the model, too.

Experimentally, it has been shown that the magnetic field in DNA molecule causes the electric current decreases at a stronger magnetic field [19]**.** Besides that, the transport property of the G4 DNA molecule can be tuned by tuning the magnetic field and temperature [22]. Therefore, this report is the result of theoretical research on the magnetic field effect on charge transport behavior on a periodic poly(dA)-poly(dT) DNA. The charge transport was studied by calculating electric current as a function of a magnetic field. The electric current at a certain voltage was calculated from transmission probabilities using Landauer-Buttiker formalism. The transmission probability as a function of electron energy at a certain voltage and magnetic field was calculated using Green's function technique. Calculation results show that at low voltage, the current decreases, and with a strong magnetic field the current starts to oscillate with the magnetic field. However, at high voltage, the voltage of several volts, up to a certain value of the magnetic field the current decreases and then starts to increase and oscillate with the magnetic field. This trend is observed in all sizes of DNA molecules investigated.

The systematics of this report is as follows: in the following section, the DNA molecule model and parameters being used as well as methods used in the numerical calculation will be discussed. The calculation results will be presented and discussed. In the final section, several conclusions will be stated.

METHOD

In this study, the structural model of poly(dA)-poly(dT) DNA molecule used consists of Watson-Crick DNA base pairs which are glued by sugar-phosphate *backbone* at their edge.

Therefore, there are four parallel lines of electron transmission along the DNA molecule. Electron transmission along the lines is represented by intra-strand hopping parameters. Besides that, an electron can also move vertically as well as diagonally to the symmetrical axes of the molecule. These two displacements were represented by vertical and diagonal hopping parameters, respectively. The DNA molecule model is placed in between two metallic electrodes. The DNA molecule model is represented with the following *tight-binding* Hamiltonian equation.

$$H=\sum_{i=1}^{L}\sum_{\tau=1}^{4}\left\{\varepsilon_i^{\tau}|i,\tau><i,\tau|+\sum_{\sigma=1}^{4}\left[t_{i,i}^{\tau,\sigma}|i,\tau><i,\sigma|+t_{i,i+1}^{\tau,\sigma}|i,\tau><i+1,\sigma|\right]\right\} \quad (1)$$

In the equation above, the index i is the base pairs and backbone numbers that have maximum L, the number of base pairs present in the poly(dA)-poly(dT) DNA molecule under investigation. The indices τ and σ are the strand numbers in the molecule, the backbones are represented by the numbers 1 and 4. Strands 2 and 3, respectively, consist of adenine (A) and thymine (T) bases. ε_i^{τ} is the onsite energy of the base or backbone at the site i and strand τ. Inter-site electron hopping, in one strand (intra-strand) and two different strands (inter-strand diagonal) are represented by $t_{i,i+1}^{\tau,\sigma}$ parameter. Electron hopping in the vertical direction to the symmetrical axis of the DNA molecule (intra-strand perpendicular) is represented by the $t_{i,i}^{\tau,\sigma}$ parameter.

In this investigation, the internal electric field is present in the DNA molecule as a result of the voltage difference between the two metallic electrodes. Therefore, the electric field considered is in the direction of the symmetrical axis of the DNA molecule (z-axis) and causes the hopping parameter of a particle with charge q which moves from site j to site i can be stated as follow [23].

$$t_{i,j}=\begin{cases}t_0\exp\left(\dfrac{qF}{Kk_BT}\left(z_i-z_j\right)\right); \text{ if } \left(z_i-z_j\right)<0\\ t_0 \qquad\qquad\qquad\qquad ; \text{otherwise}\end{cases} \quad (2)$$

where F is the electric field magnitude, z_i is the z coordinate of site i, k_R is Boltzmann constant, T is temperature, and K is the DNA dielectric constant DNA which is set to $3\text{x}10^{-4}$.

The presence of an external magnetic field in the direction of the symmetrical axis of the DNA molecule (z-axis) causes the hopping parameter of q charged particle which moves from site l to site j to become.

$$t_{j,l}=t_0\exp\left[-\frac{iqB\pi}{h}\left(x_l-x_j\right)\left(y_l+y_j\right)\right] \quad (3)$$

where h is Planck constant and x and y are the particle coordinate on the x,y plane [24].

The electric current flowing through the molecule at a certain voltage is calculated using the Landauer-Buttiker formalism [25] which states.

$$I=\frac{-e}{h}\int dET(E)\left[f_L(E)-f_R(E)\right]. \quad (4)$$

The Fermi-Dirac distribution function ($f(E)$) represents the charge density in the left and right electrodes which play a significant role in the transport process. The transmission probability at energy E is represented with $T(E)$. The transmission probability is calculated from electron Green's function (G) at the molecule and the electron energy broadening due to the presence of metallic electrodes (Γ) using relation [25].

$$T_{pq} = \mathrm{Tr}\left[\Gamma_p G_{pq} \Gamma_q G_{pq}^{\dagger}\right] \quad (5)$$

The energy broadening Γ can be calculated from self-energy Σ using the relation.

$$\Gamma_{pq} = i\left(\Sigma_{pq} - \Sigma_{pq}^{\dagger}\right) \quad (6)$$

The self-energy Σ is a consequence of the presence of a metallic electrode on the electron energy via contact between molecule and electrode. The molecule-electrode contact and the metallic electrode system are also modeled in the regime of tight-binding binding approximation. All parameters used in this study can be found in ref. [26, 23] as well as references therein.

The electron Green's function in the molecule as a function of energy E can be stated as follow.

$$G(E) = \left[(E + i\eta) - H - \Sigma\right]^{-1} \quad (7)$$

In the equation above, the total Hamiltonian of the DNA molecule is represented by H. Self-energy Σ represents the presence of metallic electrode and molecule-electrode contacts**.** The quantity η is a small and positive number.

RESULT AND DISCUSSION

FIGURE 1 shows electric current as a function of an external magnetic field in a 48 base pairs long poly(dA)-poly(dT) DNA molecule structure calculated at a temperature of 77 K and electric voltages of 0.4, 0.8, 1.2, and 1.6 volts. At a 0.4 volt of external voltage, the electric current starts decreasing and then oscillating, its value becomes smaller if it is compared to the current without a magnetic field. The decrement of the electric current occurs due to the transmission probabilities of the electron with the energy around Ferni energy in general decreasing with the magnetic field. A similar trend is also observed in the voltage of 0.8 volt case. However, in the electric voltage of 1.2 and 1.6 volt cases, electric current is observed to decrease with the magnetic field up to a certain magnetic field strength (less than 1.0 T). For higher magnetic field strength, electric current increases while oscillating with the magnetic field. Even though the trends are different, the position of the maximum and minimum of the current spectrum for different electric voltage occurs at around the same value of the magnetic field. It indicates that the presence of a magnetic field has much influence on electron states around Fermi energy, such that the change in transmission probabilities at an energy close to Fermi energy results in electric current oscillating with the magnetic field. In addition to that, at high voltage, the electron with high energy also involves in the transport process. However, the influence of the magnetic field on the current is less dominant than the electric field. The calculation result which shows the electric current decreases with the magnetic field is in agreement with the report in reference [19]. However, for a high voltage case (1.2 and 1.6

volts) the agreement is only held in the low magnetic field regime, while in the high magnetic field regime, there is no agreement found.

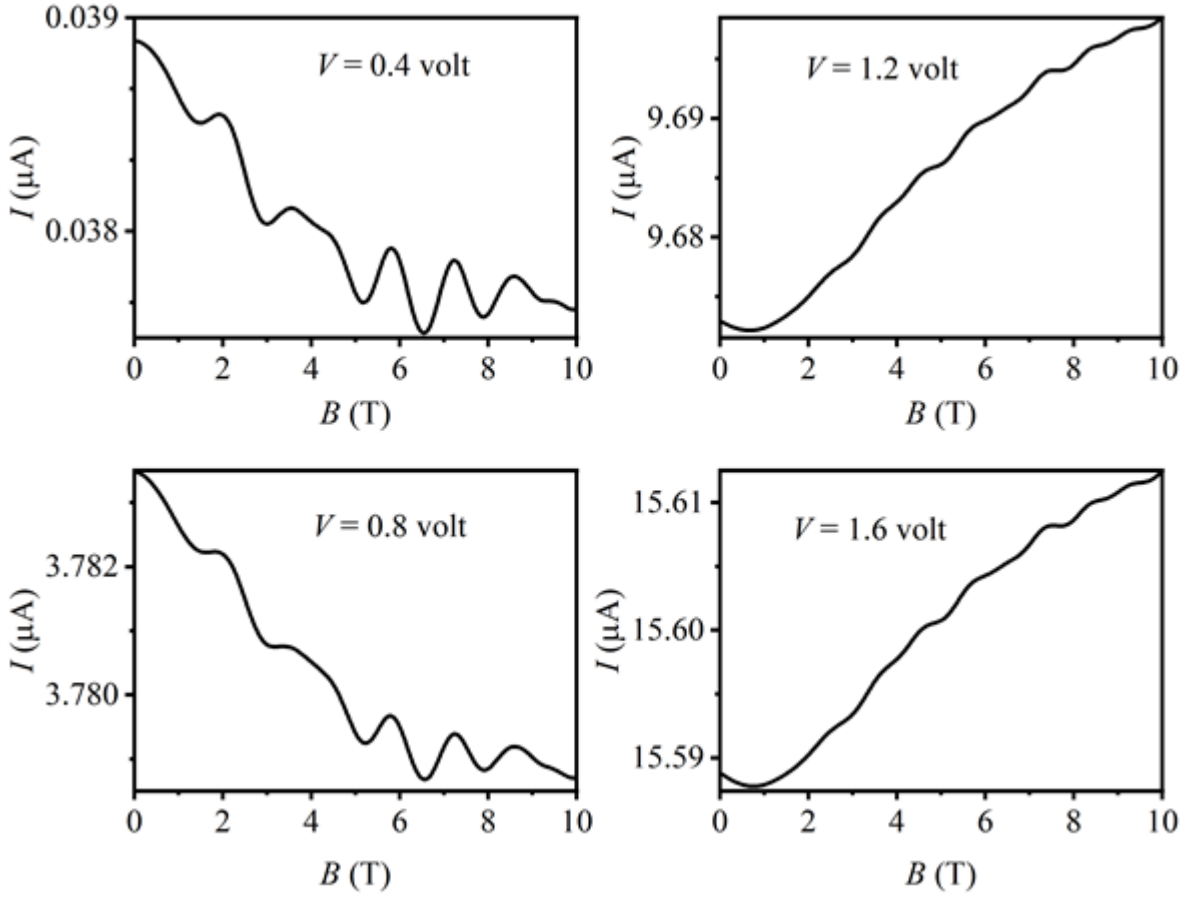

FIGURE 1. Current as a function of a magnetic field in a 48 base pairs long poly(dA)-poly(dT) DNA structure calculated at a temperature of 77 K and several electric voltages (0.4, 0.8, 1.2, and 1.6 volts).

The pattern of the electric current curve with magnetic field observed in 48 base pairs long poly(dA)-poly(dT) DNA structure, is also observed in the DNA structure of length 80 base pairs. The electric current curve as a function of an external magnetic field in 80 base pairs case calculated at the previous case temperature and the electric voltage is shown in FIGURE 2. The difference in the electric current curve pattern of the two cases can be seen from the position of local maxima and minima. It indicates that different path length taken by electron for traveling from one electrode to another electrode on an opposite site requires different magnetic field magnitude for the maximum or minimum interference to occur. Therefore, the local maxima and local minima for both cases are observed at different magnetic field magnitudes. In the two cases, it is shown that, as expected, the electric current increases with the electric voltage.

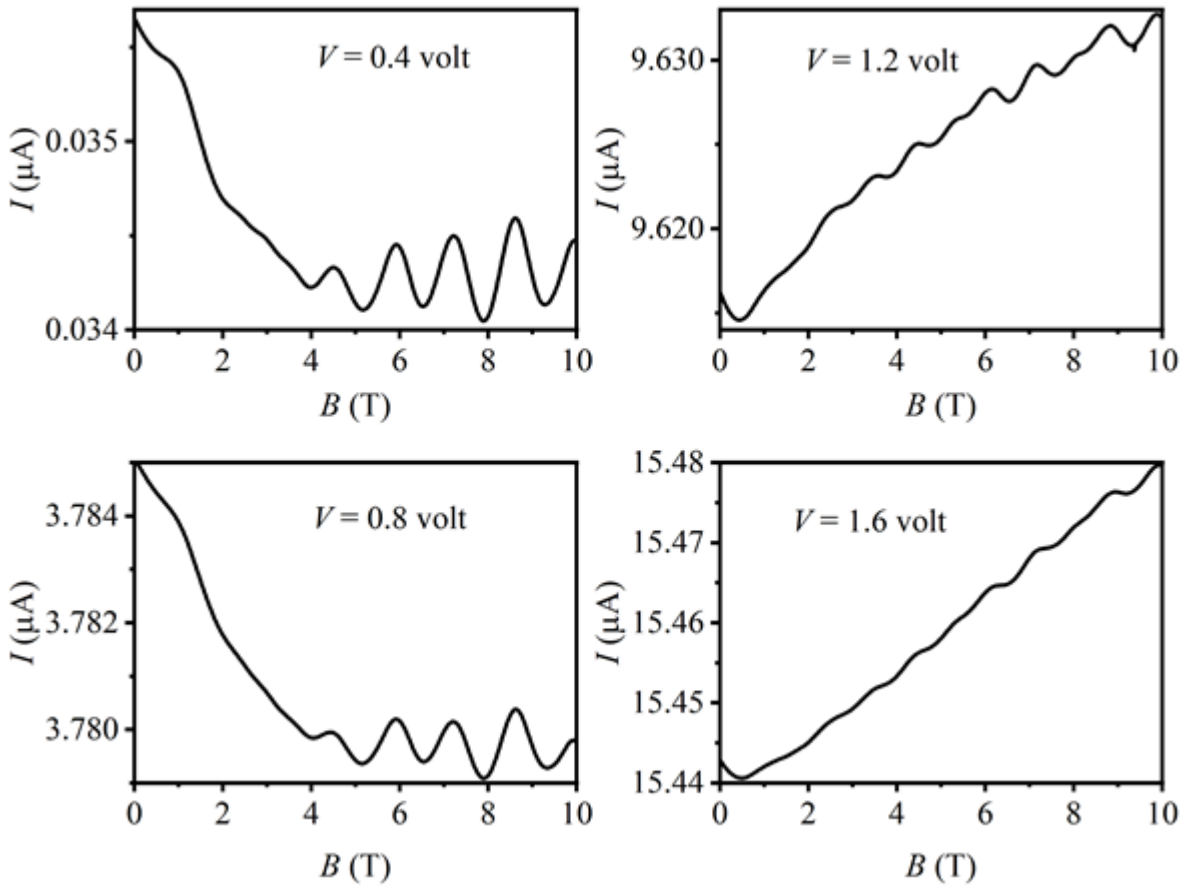

FIGURE 2. Current as a function of a magnetic field in an 80 base pairs long poly(dA)-poly(dT) DNA structure calculated at a temperature of 77 K and several electric voltages (0.4, 0.8, 1.2, and 1.6 volts).

The electric current curve as a function of magnetic fields which oscillates with the magnetic field is also observed in the current calculated molecule length of 96 and 112 base pair, as can be seen in FIGURE 3. This figure shows the electric current curve as a function of a magnetic field calculated at a temperature of 77 K and voltage of 0.4 V on several lengths of DNA structure, 40, 80, 96, and 112 base pairs. Even though the shapes of the curves are different, the four curves show there is current oscillation with local maxima and minima. The local current maximum and minimum are observed at different magnetic field magnitudes at the four curves. It supports the understanding that different pathlength requires different magnetic field magnitude for maximum or minimum wave interference to occur. Besides playing a crucial role in setting the magnitude of the magnetic field where the current reach a local maximum or minimum, the length of the molecule determines the electric current magnitude. As observed in all the voltages used, the electric current magnitude decreases with the length of the DNA molecule. Since the poly(dA)-poly(dT) molecule structure is a periodic structure, the presence of a magnetic field obliterates the periodic behavior of the structure. The longer the DNA structure, the magnetic field causes the structure becomes more disorderly in the sense of the possibility of intersite and interstrand electron hopping.

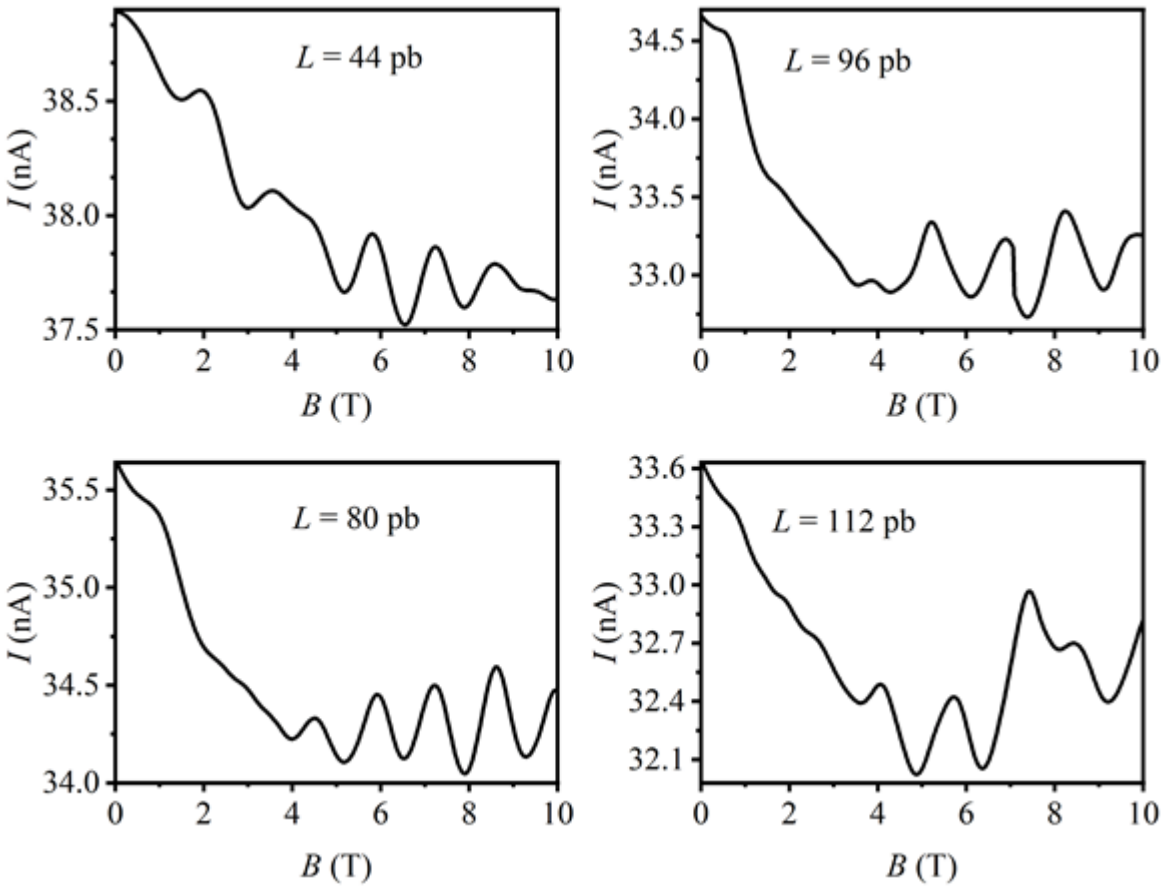

FIGURE 3. Current as a function of a magnetic field in various lengths (48, 80, 96, and 112 base pairs long) of poly(dA)-poly(dT) DNA structure calculated at a temperature of 77 K and the electric voltage of 0.4 volt.

CONCLUSION

The electric current as a function of a magnetic field has been calculated at a temperature of 77 K and voltage of 0.4, 0.8, 1.2, and 1.6 volts on a poly(dA)-poly(dT) DNA molecule with sized of 48, 80, 90, and 112 base pairs. The electric current calculated for the voltage of 0.4 and 0.8 volts shows that the current oscillates with the magnetic field. However, the current calculated for the voltage of 1.2 and 1.6 volts show the pattern of oscillation with the increment of local maxima and minima with the magnetic field. The position of local maxima and minima depends on the magnitude of the magnetic field and the DNA molecule size.

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REFERENCES

[1] D. D. Eley and D. I. Spivey, "Semiconductivity of Organic Substances, Part 9-Nucleic Acid in the dry state," *Trans. Faraday Society*, vol. 58, pp. 411-415, 1962.

[2] R. L. Zaffino, M. Mir and J. Samitier, "Label-free detection of DNA hybridization and single point mutations in a nano-gap biosensor," *Nanotech*, vol. 25, no. 10, p. 105501, 2014.

[3] D. Porath *et al*., "Direct measurement of electrical transport through DNA molecules, *Nature*, vol. 403, no. 6770, pp. 635-638, 2000.

[4] M. J. Park *et al*., "Direct measurement of the dynamics of excess electron transfer through consecutive thymine sequence in DNA," *Journal of the American Chemical Society*, vol. 133, no. 39, pp. 15320-15323, 2011.

[5] S. Nokhrin, M. Baru and J. S. Lee, "A field-effect transistor from M-DNA," *Nanotechnology*, vol. 18, no. 9, pp. 095205-095210, 2007.

[6] L. M. Bezerril *et al*., "Current-voltage characteristics of double-strand DNA sequences," *Physics Letters A*, vol. 373, no. 37, pp. 3381-3385, 2009.

[7] Ai-Min *et al*., "Enhancement of transport in DNA-like systems induced by backbone disorder," *Physical Review E*, vol. 78, no. 6, pp. 0619221-0619225, 2008.

[8] H. Yamada *et al*., "Localization properties of electronic states in a polaron model of poly(dG)-poly(dC) and poly(dA)-poly(dT) DNA polymers," *The European Physical Journal E*, vol. 17, no. 2, pp. 149-154, 2005.

[9] H. W. Fink and C. Schönenberger, "Electrical conduction through DNA molecules," *Nature*, vol. 398, no. 6726, pp. 407-410, 1999.

[10] A. Y. Kasumov *et al*., "Proximity induced superconductivity in DNA," *Science*, vol. 291,, no. 5502, pp. 280-282, 2001.

[11] Y. Zhang *et al*., "Insulating behavior of λ–DNA on the micron scale, *Physical Review Letters*, vol. 89, no. 19, p. 198102, 2002.

[12] X. F. Wang, T. Chakraborty and J. Berashevich, "Quantum transport anomalies in DNA containing mispairs," *Nanotechnology*, vol. 21, no. 48, p. 485101, 2010.

[13] Y. S. Jo, Y. Lee and Y. Roh, "Current-voltage characteristics of λ- and poly-DNA," *Materials Science and Engineering: C*, vol. 23, 841-846, 2003.

[14] D. Klotsa, R. A. Romer and M. S. Turner, "Electronics Transport in DNA," *Biophysical Journal*, vol. 89, no.4, pp. 2187-2198, 2005.

[15] S. Roche, "Sequence dependent DNA-mediated conduction," *Physical Review Letters*, vol. 91, no. 10, pp. 1081011-1081014, 2003.

[16] I. Kratochvílová *et al*., "Charge transport in DNA oligonucleotides with various base-pairing patterns," *he Journal of Physical Chemistry B*, vol. 114, no. 15, pp. 5196-5205, 2010.

[17] R. Gutiérrez, S. Mandal and G. Cuniberti, "Quantum Transport through a DNA Wire in a Dissipative Environment," *Nano Letters*, vol. 5, no. 6, pp. 1093-1097, 2005.

[18] N. B. Muren, E. D. Olmon and J. K. Barton, "Solution, surface, and single molecule platforms for the study of DNA-mediated charge transport," *Physical chemistry chemical physics*, vo. 14, no. 40, pp. 13754-13771, 2012.

[19] N. M. Khatir, Z. A. Malek and S. M. Banihashemian, "Temperature and magnetic field driven modification in the I-V features of gold-DNA-gold structure," *Sensors*, vol. 14, no. 10, pp. 19229-19241, 2014.

[20] J. R. Wong *et al*., "Magnetic fields facilitate DNA-mediated charge transport," *Biochemistry*, vol. 54, no. 21, pp. 3392-3399, 2015.

[21] D. Kang *et al*., "Magnetic field tuned charge transport in a G4-DNA molecular devices," *Journal of Physics: Condensed Matter*, vol. 23, no. 5, p. 055302, 2011.

[22] N. M. Khatir, Z. Abdul-Malek and S. M. Banihashemian, "Influences of Magnetic Fields on Current-voltage characteristics of gold-DNA-gold structure with variable gaps," *Materials Science in Semiconductor Processing*, vol. 36, pp. 134-139, 2015.

[23] F. Rahmani and E. Yudiarsah, "A study of the poly(dA)-poly(dT) DNA electric field-dependence: density of states (DOS) analysis," *IOP Conference Series: Materials Science and Engineering*, vo. 763**,** no. 1, p. 012067, 2020.

[24] A. M. Risqi and E. Yudiarsah, "Magnetic field and temperature effect on the localization length of poly(dA)-poly(dT) DNA molecule," *AIP Conference Proceedings*, vol. 2023, no. 1, p. 020012, 2018.

[25] S. M. A. Daraghma, S. Talebi and V. Periasamya, "Understanding the electronic properties of single-and double-stranded DNA," *The European Physical Journal E*, vol. 43, no. 6, pp. 1-9, 2020.

[26] K. A. Rahmi and E. Yudiarsah, "IV characteristics of a four-chain DNA model in environment disorder," *AIP Conference Proceedings*, vol. 2023, no. 1, p. 020045, 2018.