Study of Electrical and Thermoelectrical Properties of One Strand DNA Chain for Nanoscale Thermoelectric Applications

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Abstract

The concept of using DNA molecules for designing nano-scale electronic systems has attracted researcher's attention due to the unique properties of DNA, such as self-assembly and self-recognition. Thus, increased number of studies, theoretically and experimentally, have been carried out to study the possibility of adopting DNA molecules in designing nanoscale thermoelectric devices. In this work, a general expression of the electron transmission probability that describes the electron transfer through one strand DNA chain has been derived using the steady-state-formalism by assuming one strand of DNA molecules as line model. The energy-dependent transmission was studied, then energy-and temperature-dependent Seebeck coefficient, and thermoelectric characteristics of four one strand DNA sequences: $(A\text{-}A)_{10}$, $(C\text{-}C)_{10}$, $(G\text{-}G)_{10}$ and $(T\text{-}T)_{10}$ are theoretically studied. According to the obtained results, it is found that the transmission behavior (magnitude and position) is varying with the type of DNA sequence. Also, the energy dependent Seebeck coefficient (*S-E)* curves clearly show a nonlinear energy-dependence, while the relationship between Seebeck coefficient and temperature *(S-T)* is linear. Thermoelectric power factor as a function of temperature was found to be enhanced with the temperature increment for the four types of DNA nucleobases. The highest values of thermoelectric power factor belong to thymine ($120 Wm^{-1}K^{-2}$) and cytosine ($60\ Wm^{-1}K^{-2}$), that nominate them as outstanding candidate thermoelectric materials to be adopted in the fabrication of one strand DNA-base nanoscale thermoelectric devices.

Key Words: One Strand DNA, Transmission, Seebeck Coefficient, Thermoelectric Power.
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Introduction

Charge transport in DNA has gained huge attention over the last decades, not only for its importance in biological processes (Schuster, 2004), but also for physical applications, which use the DNA as molecular systems or by using its properties in self-assembling and self-recognition (Mertig & Kirsch, 1999). Instead of, DNA is working as a molecular wire in specific sequences such as a poly (GC). It also can be doped with metallic ions as in the state of M-DNA (Di Felice, Calzolari, & Zhang, 2004). Regardless of the different experimental properties and intrinsic complexities of the molecules, there is a consensus that DNA molecules sometime behave as a semiconductor with a wide band energy and close bandwidth (Cohen, Nogues, Naaman, & Porath, 2005; Porath, Bezryadin, De Vries, & Dekker, 2000; Storm, van Noort, de Vries, & Dekker, 2001; Xu, Zhang, Li, & Tao, 2004; Yoo et al., 2001). On the other hand, thermoelectricity of molecular junctions is another concept raised and proofed to

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be essential to figure out the fundamental scientific concepts of the thermoelectric effect at single-molecule level, as well as to enhance the technologies for getting electrical energy from wasted heat.

It can describe the voltage or the current generation through molecular junctions connected to two leads that have different temperatures (Aradhya & Venkataraman, 2013). Further, thermoelectricity can also be defined as a process that describes the generation of electric potential from the temperature differences or vice versa. One remarkable application of thermoelectricity is the thermo-couple that used for temperature measurement. In the thermoelectricity research, two essential research topics are currently under investigation. First topic is the generation of electricity from wasted heat, and second one is thermoelectric refrigeration, in which the tuning of thermoelectric effect is used to enhance energy efficiency and minimize pollutants. Moreover, the Seebeck coefficient, which is among the thermoelectric characteristics of the molecular junctions, has been used to identify the charge carriers type (p-type or n-type) as well as the Fermi level position of the leads with respect to the molecules HOMO or LUMO levels (Reddy, Jang, Segalman, & Majumdar, 2007). Seebeck coefficient gives positive value with a negative T(E) slope in case of a p-type transport in which the HOMO level is near E_F level. While it gives negative value with a positive T(E) slope in case of a n-type transport in which the LUMO level is near E_F level. Also, according to the Landauer formula of the Seebeck coefficient, it can be concluded that the transmission function T(E) slope can be used to describe the thermoelectric properties of the molecular junctions. The focus in this paper is to investigate the relationships between transmission-energy, Seebeck coefficient-energy, Seebeck coefficient-temperature and thermoelectric power factor-temperature of four different codes of one strand DNA which are GGGGGGGGGG, CCCCCCCCCC, AAAAAAAAAA and TTTTTTTTTT (Xiang, Wang, Jia, Lee, & Guo, 2016). We will present an analytical formulas and derivation to study the transmittance, Seebeck coefficient at the Fermi level position for four one strand DNA chains. Thus, a comparative theoretical investigation of the electrical and thermoelectric characteristics for four different one strand DNA sequences will be presented.

Method and Theoretical Formulation

In the simplest single particle tight-binding model (Al-mebir & Al-Saidi, 2020; S. A. AL-Saidi & Al-mebir, 2018; S. A. AL-Saidi, Al-mebir, & Hallool, 2019), the system was assumed to be a line system where an effective on site energy is assumed for the HOMO level of each base. In addition to the influence of the interaction between any two close neighbor sites. For a homogeneous DNA such as the Poly (G), this model should be strongly functional due to the charge transport occurring within the purine strand in the hole transport case (Cuniberti, Maciá, Rodriguez, & Römer, 2007). The schematic model that has been adopted is presented in Fig. (1).

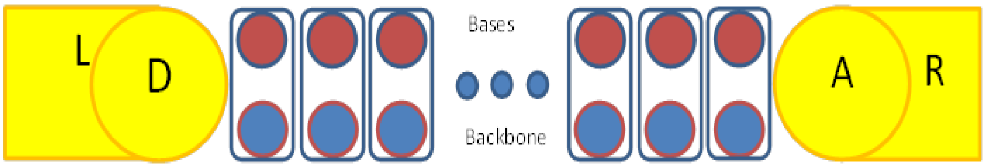


Figure 1. Illustrates the line model, in which left and right sides of the DNA(Bases) are coupled with the left lead L and right lead R in addition to D(doner) and A(accepter)

Since the electron experience a scattering from one bridge that consists of one strand of DNA. Thus, the tight-binding model can be considered to describe the DNA that is constructed as a line model. Also, since there is a single conduction gate in which sites represent bases, and every link between locations includes the existence of a coupling interaction. Therefore, the system of DNA base as single positions can be represented by the line model. In this work, our system under study that is shown in Fig. (1) can be described by using the following time-independent Hamiltonian and Dirac's notations. In this form, Hamiltonian adopts all the sub-systems interactions. The different parameters D, A, L, R and b refer to the donor, acceptor, left lead, right lead, and bridge (DNA bases with total number N). The Hamiltonian model as well the method details were already described in our previous studied (S. Al-Saidi, 2018; S.A. Al-Saidi & Al-mebir, 2020), from which we have obtained the final formula of the transmission amplitude and probability that are defined in the following forms (Datta, 2000):

$$\boldsymbol{t(E)=\frac{\overline{C}_A(E)}{\overline{C}_D(E)}} \quad (1)$$

and,

$$\boldsymbol{T(E)=|t(E)|^2} \quad (2)$$

Results and Discussion

In the following sections, electric characteristics of four different codes of one strand DNA molecule will be presented. This includes studying transmission probability properties. After that, thermoelectric properties of the proposed system will be presented including studying the dependent relationships between Seebeck coefficient and energy and temperature. Further, the thermopower factor of the proposed system will then be explained.

Transmission Probability Results

Using the tight-binding model, we can derive the transmission formula by calculating the eigenvalues expressions of DNA bases that are placed in homogenous sequence (S. Al-Saidi, 2018):

$$\boldsymbol{E_j=E_{basis}-2V_{nm}cos\left(\frac{\pi j}{N+1}\right)} \quad (3)$$

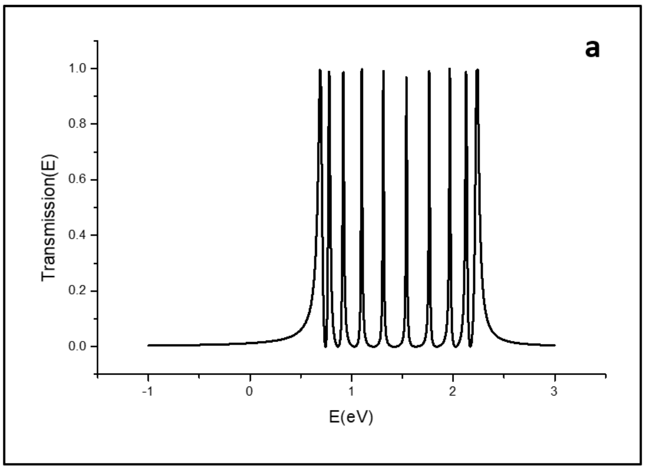
Where, E_{basis} is the energy of the base, which is given by E_G (=-2.63 eV), E_C (=-3.75 eV), E_A (=-3.25 eV) and E_T (=-4.15 eV), for the Guanine, Cytosine, Adenine and Thymine respectively (Xu et al., 2004), and are located in the LUMO energies. The interaction of coupling between closest neighbor sites refer to by V_{nm}, where V_{nm}=0.119 eV for both (G-G) and (C-C) and -0.38 eV for both (A-A) and (T-T). Where j and N refer to the single base and the total number of the bases, respectively, that are both located in the LUMO energies. So that, the density of states can be given as,

$$\boldsymbol{\rho(E_j)=\frac{N}{2\pi}\,\frac{1}{|V_{nm}|\,sin(\frac{\pi j}{N+1})}} \quad (4)$$

Considering the line model, the relationship between the transmission probability T (E) and energy E in the active region case, which contains the DNA sites only, are shown in Figs. 2 (a, b, c, d) for the sequence $(A\text{-}A)_{10}$, $(C\text{-}C)_{10}$, $(G\text{-}G)_{10}$ and $(T\text{-}T)_{10}$ respectively, using the factors V^{Ab}=- 0.1 eV and V^{bD} =-0.1 eV. It is clearly noted there are a lot of states near the active region edges own a respectively low transmission coefficient. While high transmission coefficient is presented at locations near energies of bases since the coupling between them is opened. Also, the shapes of the curves are changing with type of sequence. This was expected due to the equal values of the coupling interactions of the active region with the donor and accepter, however the energy site is dependent on the sequence. In other word, the transmission spectrum (magnitude and location) is changing with the type of sequence. This transmission spectrum is very important factor to study the transport characteristics of the electron mobility process in molecular electronic (Al-mebir & AL-Saidi, 2021). It will be used to calculate the Seebeck coefficient and thermoelectric power factor in the DNA molecule. In the off-resonance limit, the following Landauer formula can be used to relate the Seebeck coefficient of the molecular junctions at zero applied voltage with the transmission function (T(E)) in the vacancy of the Fermi level (Xiang et al., 2016):

$$\boldsymbol{S(E_F)=-\frac{\pi^2k_B^2T}{3e}\,\frac{\partial\ln(T(E))}{\partial T(E)}\bigg|_{E=E_F}} \quad (5)$$

where k_B is the Boltzmann constant, e donates the electron charge, T refers to the junction's average temperature, and E_F is the Fermi level. Therefore, the Seebeck coefficient is related to the slope of T(E) only in the vacancy of the Fermi level of the systems, where the Fermi level is located between the HOMO and LUMO energies.



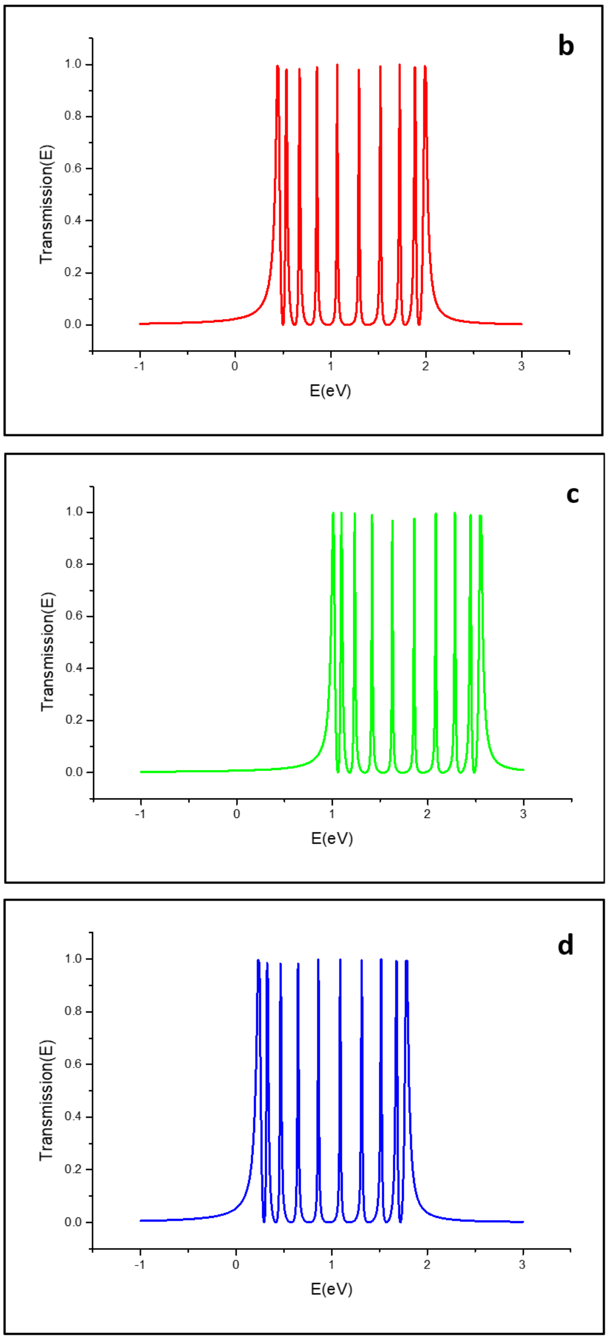
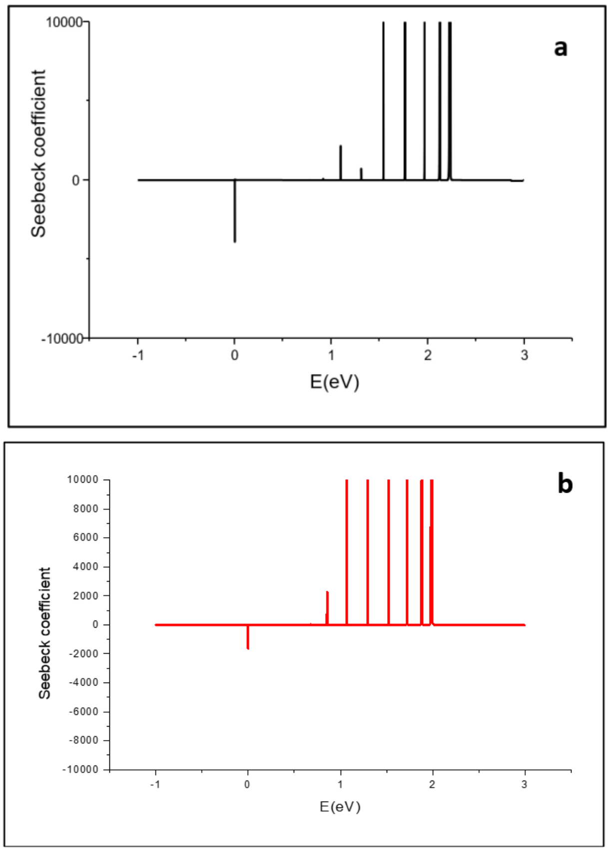


Figure 2. Transmission with respect to energy for sequence (A-A) 10 (a), sequence (C-C) 10 (b), sequence (G-G) 10 (c), and sequence (T-T) 10 (d).

Seebeck Coefficient Energy Dependent

The Seebeck coefficient reflects the capability of thermoelectrics to produce electricity from heats. And because of the correlation between all parameters, it is not an easy step to improve the thermoelectric materials efficiency. For instance, if we look at the transmission coefficient T(E) which describe the movement of electrons with energy E from one lead to the other through a molecule. We can see that the conductance and Seebeck coefficient are related to each other because they are all derived from T(E). The Seebeck coefficient (S) that is shown in Fig. 3 (a to d) is proportional to the slope of ln T(E), obtained in the vacancy of the Fermi energy E_F. Thus, the peaks dip of Seebeck coefficient as function of energy are depended on resonances of transmission coefficient which depend on number and type of bases, and the electrical conductance is proportional to $T(E_F)$. Therefore, by tuning the Fermi energy close to high transmission slope region or transmission resonance, then both conductance and Seebeck coefficient can be significantly enhanced. For this, improvement of electron transport is a must to engineer different materials for thermoelectrical applications. The results obtained for Seebeck coefficient energy dependent is in good agreement with previous studies (Noori, Sadeghi, & Lambert, 2017; Zhao et al., 2016), proposing that the essential structure of S(E) given by Eq. (25) can also mirror the self-similarity related with the apportioning of the spectrum.



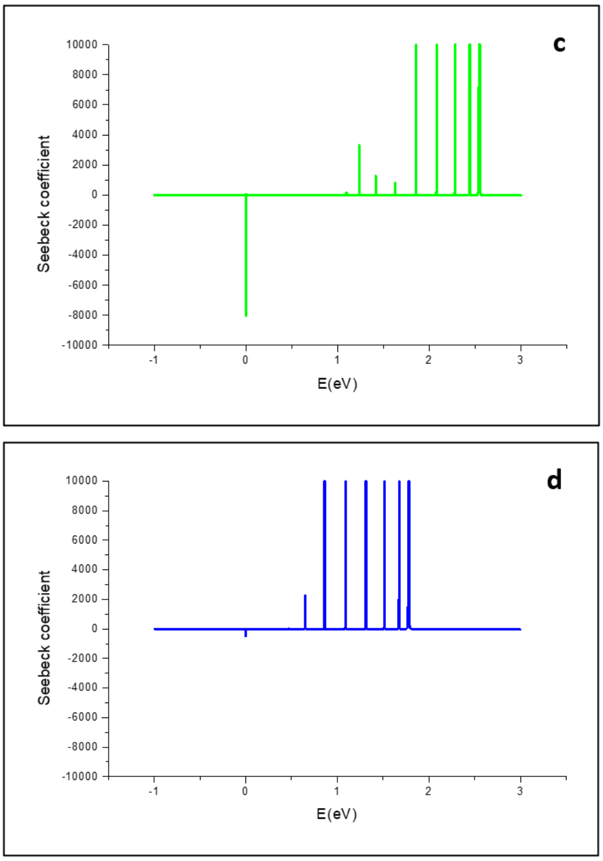


Figure 3. Seebeck coefficient with respect to energy for sequence (A-A) 10 (a), sequence (C-C) 10 (b), sequence (G-G) 10 (c), and sequence (T-T) 10 (d) for line model

Seebeck Coefficient Temperature Dependent

The conductance for the sequence (G-C) will be considered with respect to temperature. Our results for the conductance will summarize, as long as the transmission probability is obtainable in our model computation, by using the following form (Gutiérrez, Mandal, & Cuniberti, 2005):

$$\boldsymbol{G = \frac{2e^2}{h}\int_{-\infty}^{\infty} dE\, T(E)\,\frac{\partial f(E)}{\partial E}} \quad \mathbf{(6)}$$

f_α (E) refers to the function of the electrons Fermi distribution of the lead *α,* with *α=L, R,*

$$\boldsymbol{f_\alpha(E) = \left\{1 + exp\left[\frac{E-\mu_\alpha}{K_B T_\alpha}\right]\right\}^{-1}} \quad (7)$$

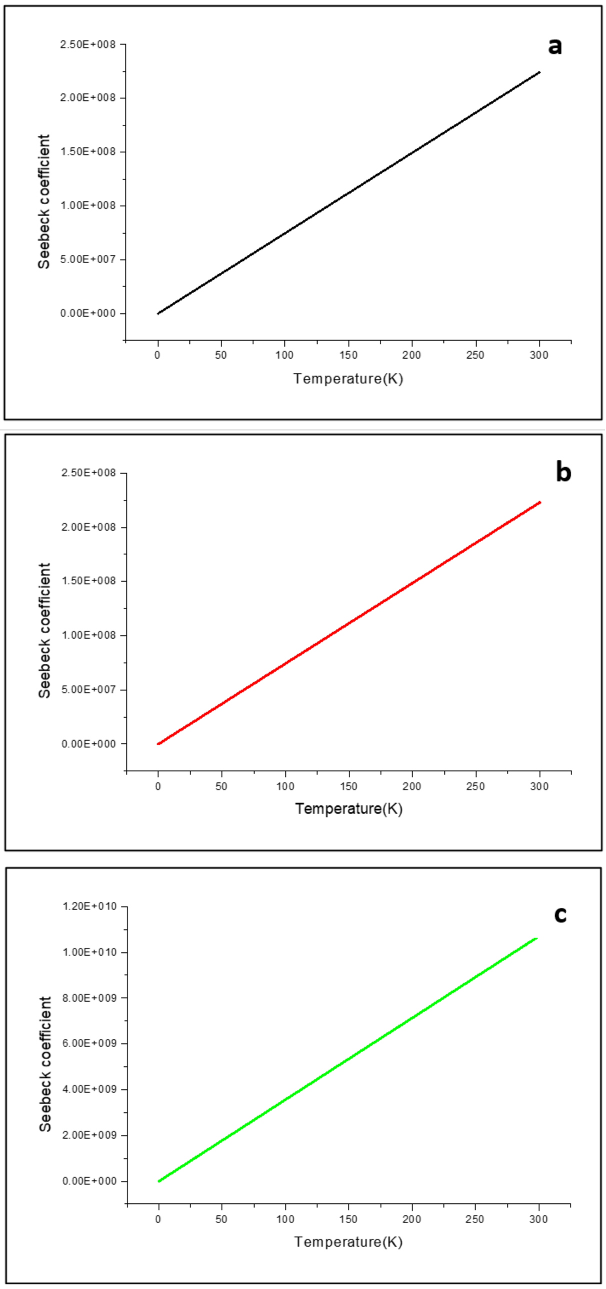
Where μ_α represents the chemical potential of the lead α, with $\mu_L = \frac{V}{2}$ and $\mu_R = -\frac{V}{2}$, where V refers to the bias voltage, while T_α refers to the temperature of the lead α.

The thermoelectric power factor is given by (Maciá, 2005):

$$\boldsymbol{p = S^2 x\, G} \quad \mathbf{(8)}$$

Where S is thermopower and G represents electrical conductivity.

Temperature Dependence of the Seebeck Coefficient results for one strand model are presented in Fig. 4 (a-d). The conductance resulted from electron transport or hopping process among the chemical potentials and energy levels of active region of neighboring locations. Fig.4 (a to d) shows the observed temperature dependent Seebeck coefficient. The relationship between Seebeck coefficient with temperature is linear where the Seebeck coefficient increase with increase of the temperature for all type of DNA nucleobases. However, there is a difference in values of Seebeck coefficient with different DNA nucleobases. This behavior is in agreement with the previous study (Babichev, Gasumyants, & Butko, 2013). This observation can be understood according to the diffusion.



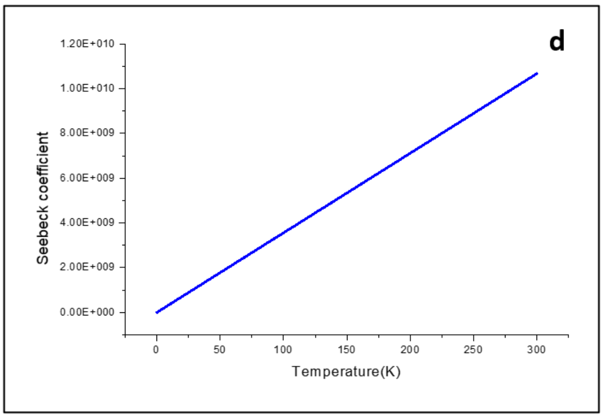
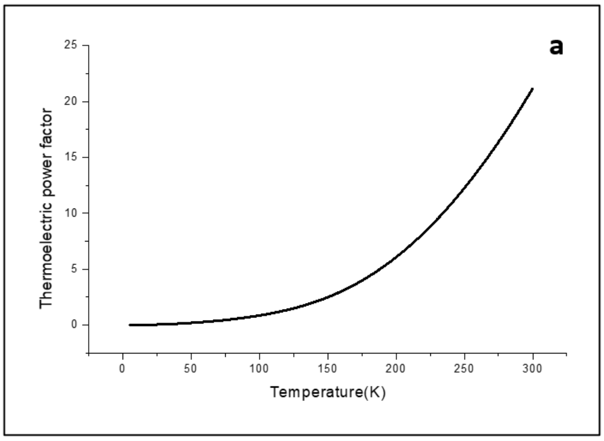


Figure 4. Seebeck coefficient with respect to temperature for line model for sequence (A-A) 10 (a), sequence (C-C) 10 (b), sequence (G-G) 10 (c), and sequence (T-T) 10 (d)

Thermoelectricity Temperature Dependent

The results of thermoelectric power factor have been studied by using Eq. (28). Fig.5 with respect to temperature. It is also noted that there is a monotonic increase in the power factor with the temperature for the four types of DNA nucleobases in same behavior. It can be noted that the highest thermopower value belongs to thymine ($120Wm^{-1}K^{-2}$) and cytocine ($60\ Wm^{-1}K^{-2}$) than other types of DNA nucleobases. This can be due to the difference in value of electrical conductivity. These results showed in a good match with previous studies M. A. Annasaheb (Maske, 2016). Thus, we can conclude that the efficiency of thermoelectric conversion is influence through changes in temperature.



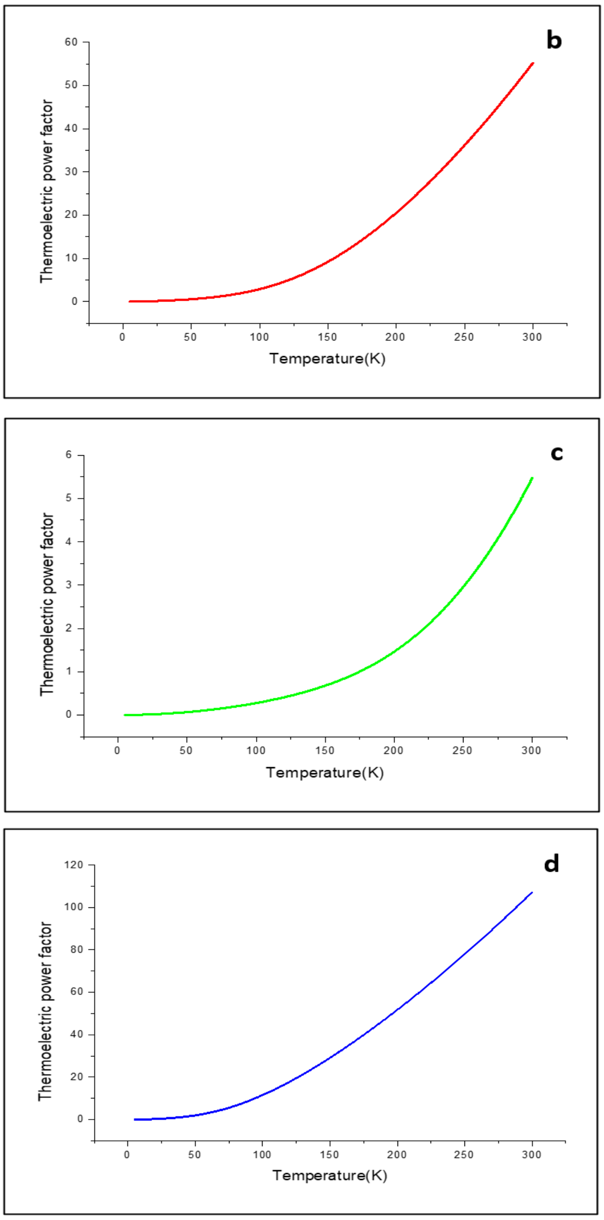


Figure 5. Thermoelectric power factor as a function of temperature for sequence (A-A) 10 (a), sequence (C-C) 10 (b), sequence (G-G) 10 (c), and sequence (T-T) 10 (d) for line model

Conclusion

Electric and thermoelectric properties of four different codes of one strand DNA molecule have been theoretically studied. The general formula of the transmission probability of electron transfer through one strand DNA chain has been derived using the steady state formalism by assuming one strand of DNA molecules as line model. The transmission spectrum (magnitude and position) varying with the type of sequence. Also, the energy dependent Seebeck (*S-E)* curves clearly show a nonlinear energy-dependence. The *S-E* peak dips are almost the same for four sequences, but they are not equal in the values or onsite energies, this difference depend on transmission that belongs to every sequences. Further, the relationship between Seebeck coefficient with temperature is found to be linear where the Seebeck coefficient increase with increase of the temperature for all type of DNA codes, however there is a difference in magnitude of Seebeck coefficient for different DNA codes. Moreover, thermoelectric power factor as a function of temperature were calculated and found to be increased with the temperature for four types of DNA nucleobases in same behavior. It was observed that the highest values of thermoelectric power factor belong to thymine ($120Wm^{-1}K^{-2}$) and cytosine ($60\ Wm^{-1}K^{-2}$) than other types of DNA nucleobases, which can be due to the difference in electrical conductivity values. Therefore, from these results it is obvious that one strand DNA molecules can have interesting characteristics that can lead to novel 1D thermoelectric materials. This can be further investigated in the future be studying the effect of DNA doping on tuning the thermopower values for improved thermoelectrical applications.

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