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Modulation of spin transport in DNA-based nanodevices by temperature gradient: A spin caloritronics approach

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ABSTRACT

Spin caloritronics, a novel and rich research field, combining spin, charge and heat transport in materials, provides alternative strategies for thermoelectric waste heat recovery, and the information technologies. Understanding of the spin transport properties of materials has important implications for spin-based devices. Flexibility, low cost, and adjustable conductance are the important factors to consider the spin transport properties of DNA chains. The spin current corresponding to spin-up and spin-down electrons in the presence of a temperature gradient along the DNA chain are calculated. $\nabla T = 1\ K/\text{Å}$ is the most appropriate temperature gradient in which the maximum spin current flows. The spin current of different sequences determines the best sequence for spin transport in different situations. Applying the external magnetic field can amplify the spin current along the DNA chain, and one can choose the most appropriate field. $I_s - V$ characteristic diagrams corresponding to different sequences are distinctive and determine the spin-dependent negative differential resistance (SNDR) regions corresponding to the negative slope intervals. Eventually, the spin-dependent Seebeck effect (SDSE) in DNA and the SDSE coefficients as a function of temperature are studied. The peak of the SDSE diagrams is different for different species of sequences. $Poly(AT)$, $hc1$, and $poly(CG)$ show maximum peaks of SDSE coefficient at 300, 310, and 320 K, respectively. Therefore, one can design a DNA based spin nanodevice with maximal efficiency in different situations.

1. Introduction

Thermoelectric (TE) devices are attractive for applications requiring the conversion of heat to work without moving parts, a task for which nanoscale systems are particularly suitable [1,2]. The thermoelectric effect can serve as an accurate probe to investigate the transport characteristics of molecular systems [3,4]. Thermoelectric materials have applications in recycling utilization of industrial waste heat and automobile exhaust heat, high-efficiency cooling of next-generation integrated circuits, and full-spectrum solar power generation [5,6]. In recent years, the fields of spin-caloritronics have gained considerable attention [7,8]. The field spincaloritronics combines thermoelectrics with spintronics and nanomagnetism, which recently enjoys renewed attention [9]. Spin caloritronics refers to research efforts in spintronics when a heat current plays a role [10]. This serves as a conceptual framework to analyze the interplay of charge, spin, and heat transport. Spin caloritronics is as old as spin electronics, starting in the late1980's with Johnson and Silsbee's [11] visionary theoretical insights into the nonequilibrium thermodynamics of spin, charge, and heat in metallic heterostructures.

The spintronics (or spin-based electronics) manifested itself with major advantages in speed, heat dissipation, and power consumption [12]. Spintronics manipulates the electron spin and its associated magnetic moment in electronic devices, which traditionally exploit just the electron charge. The most important application in the usage of electron spin can be in information theory for storing, processing and transferring the information securely and with the lowest waste. Inorganic materials such as metals and semiconductors are traditional materials for spintronics. In the meantime, molecular spintronics, in particular, proposes to use molecules to perform spintronic functions in conventional applications and beyond. The integration of molecule-based materials into building-block spintronic heterostructures, such as spin valves and magnetic tunnel junctions, as well as the realization of all-molecular devices, is of much interest. It is an important challenge to understand the key mechanisms for spin-dependent transport in molecule-based functions. Organic materials have been seriously considered in spintronics devices after experimental works on the spin-dependent electrical properties of them [13]. Selecting of any material in spintronics is based on its ability for spin

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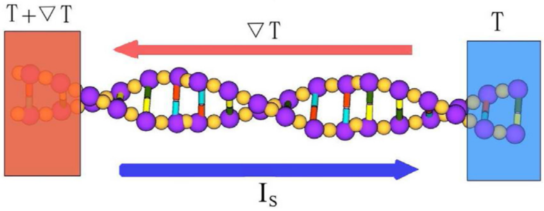

Fig. 1. The schematic illustration of the physical model of temperature gradient driven spin transport in DNA chain. Some of the right-hand side base pairs of DNA chain are in the contact of the cold thermostat at temperature T and other side is in the contact of the hot thermostat at temperature $T + \nabla T$. The temperature gradient and the spin current directions are presented.

polarization. In this direction, DNA has been taken into consideration as a potential candidate for spin polarization due to its chirality. The spin-orbit coupling originating from the helical electric field can be the source of its spin selectivity. Such a chiral-induced spin selectivity (CISS) effect has been first observed in double-stranded DNA molecules (dsDNA) [14–16]. Chiral molecules have identical composition, connectivity, and conformation but have a nonsuperimposable mirror image, so that they can exist as two different molecules or distinguishable enantiomers [17]. Chiral molecules break parity symmetry; however, they retain time-reversal symmetry, and it is necessary to have a charge flowing through them in order to break time-reversal symmetry and thus meet the symmetry requirements for generating a magnetic field along the chargeâ;;s velocity direction [18]. The recent experiments have shown that chiral organic molecules can act as electron spin filters at room temperature (CISS) [15].

In this regard, we have tried to study the reciprocal role of heat and spin transfer in DNA chains. Our main aim is obtaining the net spin current in DNA and modulating it via the applying of a temperature gradient along the chain. For this end, we have established the temperature gradient between the two ends of DNA and studied its effect on the spin transfer of chain. A schematic illustration of our physical model is presented in Fig. 1. We have used a simple theoretical model based on the combination of classical Peyrard–Bishop–Dauxois (PBD) model and quantum tight-binding approach. The PBD model can describe the dynamical motions of DNA base pairs. The nearest neighbor tight-binding approach represents the charge transport between the DNA sites with considering the electron spin and by adding the spin-orbit coupling term. The most considerable phenomenon which can discuss is the spin-dependent Seebeck effect (SDSE) that can convert thermal energy into spin current. Our aim is to study the spin-Seebeck transport along DNA chain driven by the thermal bias, and understand how the characteristics of DNA influence its thermal induced spin-Seebeck transport. A thermally driven spin-Seebeck transport in chiral DNA-based molecules can provide useful information in the standard current-voltage studies and can demonstrate the possibility of making spin-based thermoelectric devices for spin caloritronic devices based on DNA molecules.

The paper is organized as follows. In Section 2 we introduce the system under study, the Hamiltonian model, and the obtained evolution equations. In Section 3 we present our results for spin-dependent currents, temperature gradient effect, external magnetic effect, $I_s - V$ characteristic diagram, and spin-dependent Seebeck effect.

2. Model and methods

Using a semiclassical approach, a simple and effective Hamiltonian for spin transport through the DNA chain can be proposed as

$$H_{mol} = H_0 + H_{so},$$

where

$$H_0 = H_{DNA} + H_{Charge} + H_{DNA-Charge}, \tag{1}$$

$$\begin{aligned} H_{so} = \sum_n [& 2it_{so}\cos\theta (c_n^{\dagger\uparrow} c_{n+1}^{\uparrow} - c_n^{\dagger\uparrow} c_{n-1}^{\uparrow} \\ & - c_n^{\dagger\downarrow} c_{n+1}^{\downarrow} + c_n^{\dagger\downarrow} c_{n-1}^{\downarrow}) \\ & + D_{n,n+1} c_n^{\dagger\uparrow} c_{n+1}^{\downarrow} - D_{n,n+1}^{*} c_n^{\dagger\downarrow} c_{n+1}^{\uparrow} \\ & + D_{n-1,n}^{*} c_n^{\dagger\downarrow} c_{n-1}^{\uparrow} - D_{n-1,n} c_n^{\dagger\uparrow} c_{n-1}^{\downarrow}], \end{aligned} \tag{2}$$

$$H_{DNA} = \sum_n [\frac{1}{2} m\dot{y}_n^2 + V(y_n) + W(y_{n+1}, y_n)], \tag{3}$$

$$H_{Charge} = \sum_n \sum_\sigma [\epsilon_n c_n^{\sigma\dagger} c_n^{\sigma} - V_{n,n+1}(c_n^{\sigma\dagger} c_{n+1}^{\sigma} + c_{n+1}^{\sigma\dagger} c_n^{\sigma})], \tag{4}$$

$$H_{DNA-Charge} = \chi \sum_n y_n c_n^{\sigma\dagger} c_n^{\sigma}. \tag{5}$$

Here H_0 is an extended Peyrard-Bishop-Holstein (PBH) Hamiltonian which represents the transport of a charge with spin σ in DNA molecules [19]. H_{DNA} is the DNA lattice Hamiltonian described by the nonharmonic PBD model [20], where, m is the mass of base pairs, y_n is displacement of DNA base pairs along the Hydrogen bonding, $V(y_n) = D_n(e^{-a_n y_n} - 1)^2$ is the Morse potential provides the effective interaction between complementary bases with a_n as the width of the Morse potential and D_n as its depth. $W(y_{n+1}, y_n) = \frac{k}{2}(1 + \rho e^{-b(y_{n+1}+y_n)})(y_{n+1} - y_n)^2$ is the stacking interaction of neighboring base pairs in the chain, where k is the coupling constant, ρ is the stiffness parameter, and b is the damping coefficient. H_{Charge} is the charge carrier Hamiltonian, where $c_n^{\sigma\dagger}$ and c_n^{σ} are the creation and annihilation operators of an electron with spin σ, respectively, and ϵ_n is the on-site energy for each base pair. The charge hopping is restricted to nearest-neighbor base pairs and given by $V_{n+1,n}$. where $V_{n+1,n} = V_0[1 - \beta_n(y_{n+1} - y_n)]$ would be dependent on the relative distance between two consecutive molecules on the chain [21]. $H_{DNA-Charge}$ is the mutual interaction between the DNA lattice and charge, where χ is the coupling between the charge and DNA. H_{so} is considered as a Rushba-like spin-orbit interaction in the second quantization representation, while an electron with spin σ moves in a helical DNA molecules [22], where $D_{n,n+1} = it_{so}\sin\theta\{\sin[n\Delta\phi] + \sin[(n+1)\Delta\phi] + i\cos[n\Delta\phi] + i\cos[(n+1)\Delta\phi]\}$. Also, t_{so} represents the spin–orbit coupling constant, θ is the helix angle and $\phi = n\Delta\phi$ is the cylindrical coordinate with ϕ the twist angle. On the other hand, preservation of time reversal symmetry leads to $D_{n,n-1} = D_{n-1,n}^{*}$.

We have tried to use the nonlinear dynamical systems theory for analyzing the system. Therefore, the evolution equations of the classical part of system are derived via the Hamilton equation $\dot{p} = -\frac{\partial H}{\partial \dot{q}}$, where p is the generalized momentum, H is the Hamiltonian, and q is the generalized coordinates. The evolution equation of classical displacement of the base pairs are written as:

$$\begin{aligned} \ddot{y}_n = & \frac{2a_n D_n}{m} e^{-a_n y_n}(e^{-a_n y_n} - 1) \\ & + \frac{kb\rho}{2m}[e^{-b(y_n+y_{n-1})}(y_n - y_{n-1})^2 + e^{-b(y_{n+1}+y_n)}(y_{n+1} - y_n)^2] \\ & - \frac{k}{m}[(1 + \rho e^{-b(y_n+y_{n-1})})(y_n - y_{n-1}) \\ & - (1 + \rho e^{-b(y_{n+1}+y_n)})(y_{n+1} - y_n)] \end{aligned}$$