Effect of Temperature on Polaron Dynamics in Poly-DNA

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Charge transport in DNA is of great importance because of both biochemical and physical reasons [1]. It has been suggested that the carriers are charged polarons[2], which are localized self-trapping states due to strong π electron-base (e-b) interactions in DNA.

We investigate the effect of temperature on polaron dynamics in the framework of a tight-binding model, in which the base pair vibration is taken into account [3]. A DNA molecule is treated as a microcanonical assembly, which means that the total energy of the system is conserved during the evolution of the base pairs and the electronic states [4]. The temperature effect is introduced as dynamical base pair fluctuations.

Polaron stability at finite temperatures is studied at first. The dissociation of a polaron will become fast with the increase of temperature. There exists a crossover of the charge localization time from strong to weak temperature dependent. The characteristic time for a polaron to conserve before it vanishes exponentially decreases with temperature T, as e^{-T}.

The polaron motion under a driven field at a finite temperature is also studied. It is found that, instead of the uniform motion at zero temperature, a polaron moves un-uniformly at a finite temperature, which indicates a discrete hopping between base pairs. A high temperature will result in a fast movement of a polaron under a deriving field, which indicates that the polaron motion is thermally activated. Thus, DNA conductivity is considered to be increased with the increase of temperature, which is coincident to some experimental findings [2].

The thermally induced base pair fluctuations affect apparently on both the stability and the motion of a polaron. It is found that the energy deviation of on-site energy and hopping integral at room temperature are about 0.21eV and 0.02eV, which are 84% and 8% of the average hopping integral. The thermally induced disorder is non-negligible.

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