THERMOELECTRIC EFFECT IN DNA BASED MOLECULAR DEVICES

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The measurement of thermoelectric voltage over a molecule with two contacts at different temperature can provide new insights into electron transport in molecular systems. In fact, the extreme sensitivity of thermopower to finer details in the electronic structure allows one to gain valuable information regarding the location of the Fermi energy relative to the molecular levels. Thus, the thermoelectric voltage over guanine (G) molecules on a graphite substrate was measured by Poler et al. using a STM tip [1]. The obtained Seebeck coefficient value ($S \approx +20\mu VK^{-1}$ at room temperature) indicates a p-type conduction. A similar figure has been recently derived in a theoretical study considering a Phenyl-dithiol molecule chemisorbed on a gold surface. In addition, this study reveals that thermoelectric voltage should be relatively insensitive to the quality of the tip contact [2]. This result deserves further attention since strong contact effects are expected in the measurement of both electrical conductance and I-V curves of DNA molecules connected to metallic leads [3].

In this work we present a theoretical study of the thermoelectric power for several oligonucleotides of increasing complexity degree, described within the tight-binding approach. In order to perform a systematic comparative study, we start by considering the thermoelectric properties of single nucleotides G, C (cytosine), A (adenine) and T (thymine), dinucleotides and codon trinucleotides of biological relevance and, finally, a representative GACT tetranucleotide. To evaluate the thermoelectric voltage we make use of the transmission as a function of energy, according to the approach introduced by Paulsson and Datta [2]. To compute the transmission coefficient at zero bias the oligonucleotides are connected to two semi-infinite electrodes [3,4]. In this way, we obtain closed analytical expressions describing the temperature dependence of the Seebeck coefficient for a complete series of short DNA chains. By the light of the obtained results, the possible use of DNA based thermoelectric devices is discussed in the context of current search for novel thermoelectric materials based on aperiodic arrangements of matter [5].

References:

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