Graphene Nanoribbons Thermopower as a Tool for Molecular Spectroscopy

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Abstract

Recent reports predict interesting changes of the electronic and thermoelectric properties of graphene-based systems, as a function of its dimensionality. The possibility of modulating and enhancing their physical responses as a function of gate potentials, disorder, defects, and other types of electronic confinement makes these systems good candidates for new technological applications [1].

One possible application is concerned with the capability of graphene-based materials to detect molecules attached to the systems, such as nitrogen dioxide and trioxide, water, and different aromatic molecules. Nitrogen-based molecules act like electron acceptors or donors, depending of their size and internal structure, changing the local carrier concentration of the graphene. Step-like modifications in the resistance of the system are then detectable at room temperature, even at a very low concentration of molecules. On the other hand, aromatic molecules are easily detected by a graphene base device due to the strong binding between graphene π-bonds and molecular aromatic rings. Actually, graphene sensibility is better than any material currently used in gas sensor devices [2].

In previous works [3], we have addressed the effects on GNRs conductance of organic molecules adsorbed at the ribbon edge. All the considered molecule distributions were ordered configurations. We found that the corresponding molecule energy spectrum is obtained as a series of Fano antiresonances in the conductance of the system, and we proposed that GNRs could be used as spectrograph-sensor devices. In this work, we calculate the thermopower of armchair graphene nanoribbons (AGNRs) in the presence of linear polyaromatic molecules (LPHCs) attached to the ribbon edges (Fig.1). We calculate the Seebeck coefficient and the electronic transmission of the systems, for different molecular configurations, taking into account one molecule, a finite number of equidistant molecules and also random distributions of molecules, which certainly is a best choice for the proposed experimental scenario. We have found that the thermopower response is enhanced by the presence of the molecules. Our results show that thermopower reflects the molecular spectra for all considered temperatures, even in the case of random molecular configuration (Fig. 2).
This evidence suggests possible novel applications for molecules detection based on thermoelectric properties of graphene nanoribbons [4].

References

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Figure 1. - Schematic view of a hybrid system composed of an armchair nanoribbon (order N and width W) and M organic molecules with L hexagons pinned at the edge of an N-AGNR.

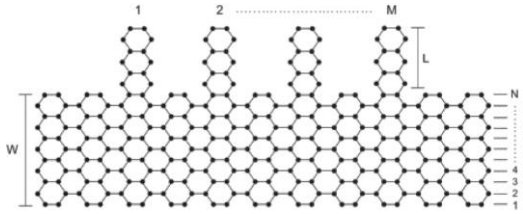

Figure 2. - Transmission and Seebeck coefficients as a function of the chemical potential for an 8-AGNR in the presence of a random distribution of molecules. Panels represent the transmission and thermopower for (a) 0.5% and (b) 3% concentrations of tetracene attached molecules, for different temperatures. The red dashed line on Seebeck coefficients curves shows the case of one molecule.