

"Vibration assisted electron tunneling processes through nano-gaps in graphene nano-ribbons for amino-acids recognition"

The rising importance of proteomics, i.e. the study of the proteins content and their functionality within a cell, requires the challenging task of protein sequencing with reliable, fast and cheap methods. Current methods are time consuming and represent a serious bottleneck for the task of massive mapping of proteins in conjunction with their functionality. Solid-state nanopores and nano-gaps have been proposed to this aim. The physical and chemical properties of graphene nano-ribbons make them particularly suited to obtain amino-acids recognition with atomistic resolution. The ability to obtain peptide bond recognition has been demonstrated theoretically at the DFT-NEGF level of the theory where just elastic scattering is considered and the main quantity is the transmission coefficient at each energy. Here we consider the inelastic scattering induced by both local vibrational modes and phonons of the electrodes to evidence the importance of such phenomena depending on the bias. To this aim, the lowest order approximation (LOE) to the self consistent Born approximation is applied.

We evidence the existence of peculiar bias regions where the differential conductivity change arises from the electrodes only or from the amino-acids side chains.