Transverse tunneling current signals across nano-gaps in graphene nano-ribbons for peptide bonds sequencing

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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, indeed, are time consuming and represent a serious bottleneck for the task of massive mapping of proteins in conjunction with their functionality. To this aim, solid-state nanopores and nano-gaps are emerging as promising tools for single molecule analysis. Due to the electronic properties of graphene, arrays of nano-gaps made on graphene nano-ribbons, are potentially, particularly suited to obtain amino-acids recognition with atomistic resolution by measuring the tunneling transverse current flowing, at a given bias, across the nano-gaps. Specific amino-acids and peptide bonds fingerprints are predicted in the context of ab-initio calculations based on the Density Functional Theory, in conjunction with the Non Equilibrium Green Function (NEGF) method and the Landauer-Büttiker approach. We have examined the peptide bond fingerprints of various types depending on the polar or charge nature of the bonded residues. From the quantum atomistic modeling reported, the proposed nano-device shows the needed selectivity and atomistic resolution properties to approach single residue recognition in peptides and proteins.