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Impact of aperture shape in force profile of ssDNA pulling through graphene nanopore: Steered molecular dynamics simulation

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ABSTRACT

Graphene nanopore based technology is one of the promising candidates for DNA sequencing as a free label, free amplification and real-time method. Many parameters like ions concentration, numbers of graphene layers, effects of electric field and nanopore size influence on the dynamic of DNA translocation. In this paper we investigate one of the ignored key factors, i.e., pore shape on pulling force profile, moving fashion of ssDNA, potential of mean force (PMF) and orientations of DNA bases, for four nucleotides, including Adenine, Guanine, Cytosine and Thymine, by steered molecular dynamic (SMD) simulation.
Our results proposed the strong effect of the pore shape on the dynamic of DNA translocation through graphene nanopore and the aperture shape should control precisely for DNA sequencing at single nucleotide resolution in experimental approaches.

1. INTRODUCTION

Graphene is a two-dimensional sheet of carbon atoms bonded by sp2 hybrid orbitals8, the graphene membrane thickness is analogous to the distance between neighboring nucleotides in DNA (0.32–0.52 nm), which makes it a perfect candidate for

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DNA sequencing by this approach. In recent years, several molecular dynamics studies were performed to complement experimental observation and to characterize the effect of applied voltage[1-5], DNA conformation[1], sequence [1-4], pore charge1, pore size[1-3,5,] pore shape[3], membrane thickness[2-4], salt concentratio[2,5,6] and effects of electric double layer[4] in ionic current blockades. In other work6 the effects of harmonic constant and pulling velocity were studied on force profile in steered molecular dynamics (SMD) simulation, via pulling ssDNA through graphene nanopore. In this study, the effects of pore shape as well as 5 layer graphene polyhedral crystal (5L-GPC) shape of nanopore were investigated for SMD simulations to indicate the impact of the graphene nanopore shape in the pulling force profile and available conformations of nucleotides in translocation. Figure 1 shows different shapes of graphene aperture that were used in this study including monolayer graphene membrane and five layers graphene polyhedral crystal (5L-GPC) shape of nanopore. Moreover the potential of mean force (PMF) calculation (using Jarzynski's equality) were carried out to investigate the free energy barrier against nucleotide in different shapes of nanopores. Figure 2 shows the schematic presentation of the system used in the project.

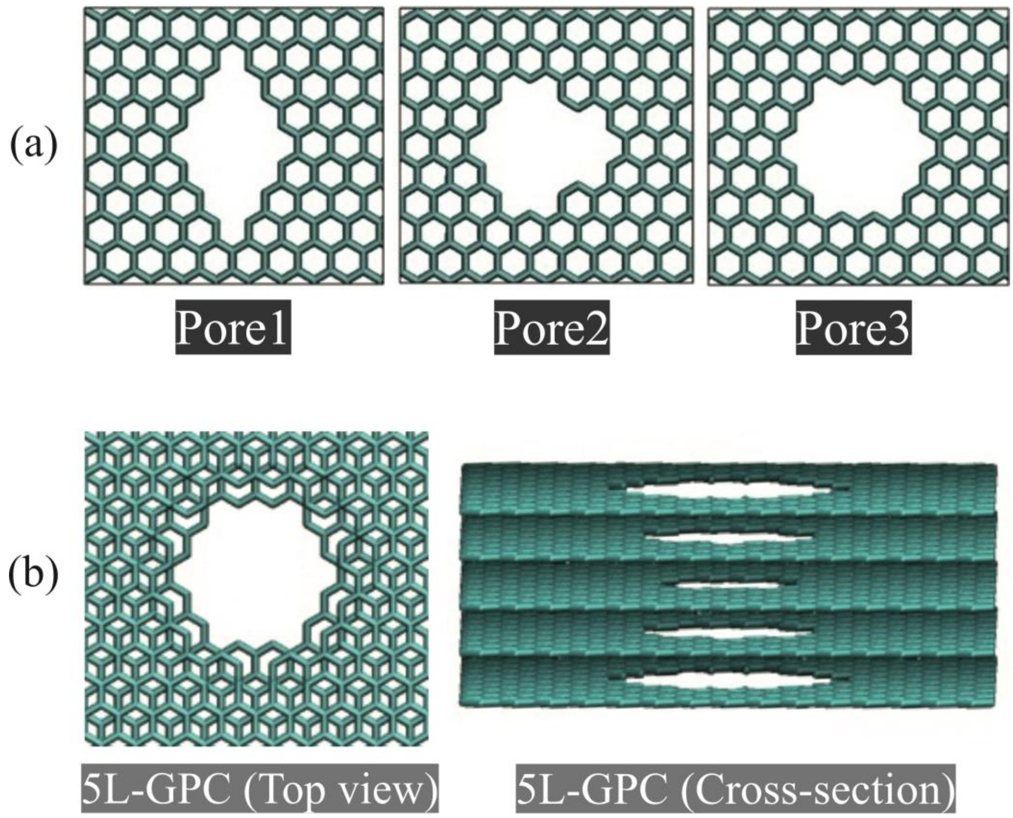

Figure 1- Different shapes of graphene aperture were used in this study. (a) Monolayer graphene membrane, (b) Nanopore with five layers graphene polyhedral crystal (5L-GPC).

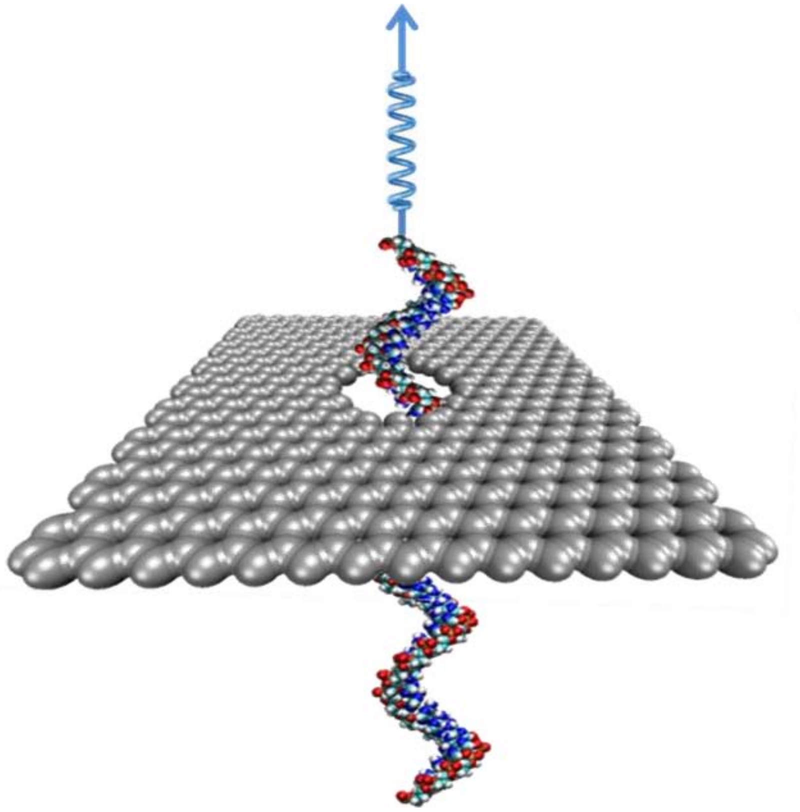

Figure 2- The schematic presentation of the system.

2. Results and Discussion

The results were shown high impact of aperture shape of monolayer and multilayer graphene on the peak values of the pulling force profile, PMF as a relative free energy barrier against nucleotides in pulling procedure within different shapes of graphene nanopores and orientation of DNA bases as nucleotides available conformations. Also Fourier transform of puling force profiles were demonstrated the specific signature of pore shape.

3. CONCLUSIONS

In summary, the effect of aperture shape was investigated in pulling process of ssDNA through graphene nanopores using steered molecular dynamics simulations.

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