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Transverse Conductance of DNA Nucleotides in a Graphene Nanogap from First Principles

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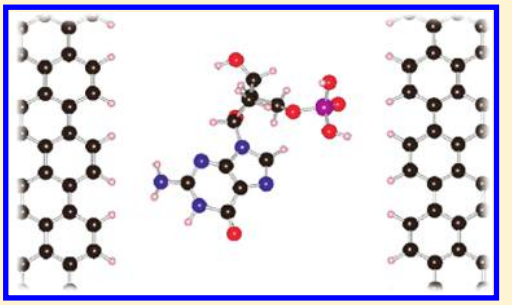
Supporting Information

ABSTRACT: The fabrication of nanopores in atomically thin graphene has recently been achieved, and translocation of DNA has been demonstrated. Taken together with an earlier proposal to use graphene nanogaps for the purpose of DNA sequencing, this approach can resolve the technical problem of achieving single-base resolution in electronic nucleobase detection. We have theoretically evaluated the performance of a graphene nanogap setup for the purpose of whole-genome sequencing, by employing density functional theory and the nonequilibrium Green's function method to investigate the transverse conductance properties of nucleotides inside the gap. In particular, we determined the electrical tunneling current variation at finite bias due to changes in the nucleotides orientation and lateral position. Although the resulting tunneling current is found to fluctuate over several orders of magnitude, a distinction between the four DNA bases appears possible, thus ranking the approach promising for rapid whole-genome sequencing applications.



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The prospect of finding an improved method for whole-genome analysis is driving significant research efforts to reach that goal. Over the past decade, the traditionally used Sanger method has been increasingly transformed into a highly parallelized and automated process, enabling the rapid rise in decoded DNA sequences seen today. Effectively, the $10000-genome has been reached through this next-generation sequencing technology. However, for a truly widespread deployment of DNA sequencing (e.g., in clinical trials and eventually even for so-called personal medicine), cost and complexity of the sequencing process will have to be reduced even further, in order to arrive at a cost of $1000 or less per genome.

In an attempt to realize such third-generation sequencing technology,[1] nanopores have been at the center of the research focus. Initially, only monitoring of the ionic current through biological pores was considered, and the merits of this approach continue to be actively investigated.[2] However, solid-state nanopores have become more and more attractive for the purpose of DNA sequencing,[3−7] since they generally provide better stability and can be more easily controlled[8] than biological pores. Furthermore, instead of measuring the ionic current, it was suggested to outfit solid-state nanopores with embedded electrodes and instead monitor the transverse tunneling current induced by them. This possibility was at first only explored theoretically,[9−12] because the technical challenges to outfit the nanopore with sufficiently thin embedded electrodes had prevented its actual fabrication until very recently.[13]

About a year ago, a new suggestion was put forward[14] to use graphene nanogaps in a double function as both separating membrane and electrodes, solving the problem of alignment and making the electrodes atomically thin[15,16] for optimal single-base resolution. (For a discussion of possible fabrication techniques to make such nanogaps in graphene, we refer the reader to ref 14 and references therein, as well as to ref 17) Even more recently, it was experimentally demonstrated for graphene nanopores[18,19] that it is possible to detect translocation events of DNA.[20−22] Furthermore, at least one density-functional-theory-based study explored the capabilities of a graphene nanopore setup for the purpose of distinguishing between nucleotides.[23] In our investigations, we have used state-of-the-art first-principles methods to study the transport properties of nucleotides inside a graphene nanogap, to assess whether or not this setup could be useful for the purpose of DNA sequencing.

To this end, we investigated the tunneling transport properties of the four nucleotides deoxyadenosine monophosphate (dAMP), deoxythymidine monophosphate (dTMP), deoxyguanosine monophosphate (dGMP), and deoxycytidine monophosphate (dCMP) when located between graphene electrodes with armchair edges chemically passivated by hydrogen.[24] The system is divided into three regions: the left and right electrodes, and the

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