OC44-T8

Transport properties of nucleotides in a graphene nanogap for DNA sequencing

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Mass-application of whole-genome information in healthcare requires a setup for fast and inexpensive DNA sequencing. In an attempt to improve sequencing technology, nanopores are being discussed as a promising tool to determine the order of nucleotides along a DNA strand. While it was originally thought that monitoring the blockage of the ionic current through a nanopore (which possesses a diameter of only a few nanometers) could lead to the determination of the base sequence, it was eventually found that this approach is unlikely to yield sufficiently accurate data for the purpose of base identification. Hence, focus shifted towards using transverse conductance properties of DNA as the key parameter for identifying and distinguishing the four types of nucleobases. Earlier this year, it was suggested[1] to use graphene nanogaps in a double function as both separating membrane and transverse electrodes, solving the problem of alignment and making the electrodes atomically thin for optimal single-base resolution. Recently, three research teams demonstrated experimentally that is is possible to translocate DNA through a graphene nanopore and record the associated drop in ionic current.[2-4] Here, we have employed *ab initio* computational simulations (using density functional theory and non-equilibrium Green's function method) to study the structure and electron transport properties of nucleotides located inside a graphene nanogap. Our setup considered different orientations of the bases with respect to the graphene electrodes. We find that, even when taking into account current changes due to base fluctuations, each nucleotide possesses a different characteristic current magnitude, owing to its distinctive electronic properties. Based on our results we thus conclude that a graphene nanogap could in principle be sufficiently sensitive to distinguish between the four nucleotides and achieve the goal of rapid and economical DNA sequencing.

References

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