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Graphene Nano-Electrodes for DNA Sequencing: an Ab initio Perspective R.H. SCHEICHER, J. PRASONGKIT, A. GRIGORIEV, Uppsala University, Y. HE, M. LIU, Institute of Microelectronics, Chinese Academy of Sciences, R. AHUJA, Uppsala University — The proposal was made that a graphene nanogap could be used to probe the transverse conductance of individual nucleotides in DNA to rapidly identify the associated base sequence. Experimentally, the characteristic drop in ionic current associated with translocation events of DNA passing through a graphene nanopore was measured. Using first-principles methods, we evaluated the performance of two graphene nano-electrodes configurations for nucleobase identification. In the first study, Nano Lett. 11, 1941 (2011), we investigated the electronic transport properties of the four nucleotides when located in a graphene nanogap by employing density functional theory and the non-equilibrium Green's function method. In particular, we determined the electrical current variation at finite bias due to changes in the nucleotides orientation. Our second study, Adv. Funct. Mater. 21, 2674 (2011), utilized molecular dynamics simulations in conjunction with electronic transport calculations to explore specifically the effect of the hydrogenated graphene edges on the translocating DNA. It is found that edge-hydrogenated graphene electrodes facilitate the temporary formation of weak H-bonds with suitable atomic sites in the nucleotides.

R. H. Scheicher
Uppsala University

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