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Edge-functionalization aspects in DNA sequencing with graphene nano-electrodes

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Slowing down DNA translocation and achieving single-nucleobase resolution are major issues for the realization of nanopore-based sequencing [see, e.g., our review in J Mater Sci 47, 7439 (2012)]. On the one hand, complex functionalization of nanopore-embedded gold electrodes with one [J Phys Chem C 112, 3456 (2008)] or two types of molecules [Appl Phys Lett 100, 023701 (2012)] might address both these issues simultaneously, but is difficult to implement in practice. On the other hand, the fabrication process of nano-gaps or -pores in graphene could readily introduce more simple edge-functionalization in the form of hydrogen atoms saturating the dangling bonds resulting from cutting the carbon network. — A range of computational tools can be used to theoretically determine the electronic structure and quantum transport properties of individual nucleotides or short DNA strands in realistic models of nanopore-based sequencing device setups. In this manner, we were able to explore the effects of the temporary formation of weak H-bonds between hydrogenated graphene edges and suitable atomic sites in the nucleotides on the dynamical [Adv Funct Mater 21, 2674 (2011)] and static [Nano Lett 11, 1941 (2011)] properties of this system. Recently also more ambitious functionalization schemes for graphene edges [arXiv:1202.3040] as well as a promising bilayer graphene setup [arXiv:1206.4199] were investigated by us. Finally, there might be a particular appeal to use graphene edges terminated with nitrogen atoms, and we have studied some of the benefits that this type of edge-functionalization could offer for the purpose of DNA sequencing. — Funding provided by the Swedish Research Council (VR), the Swedish Foundation for International Cooperation in Research and Higher Education (STINT), and the Carl Trygger Foundation for Scientific Research.