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 whole-genome sequencing [1]. Besides approaches that can directly target the forces acting on a DNA molecule [2,3], chemical modifications of the nanopore interior represent a promising method to both lower the translocation speed and simultaneously improve sensitivity. Complex functionalization of nanopore-embedded gold electrodes with one [4] or two types of molecules [5] has been theoretically explored in this regard, but it may be too difficult for practical implementation. Graphene nanopores or nanogaps might be better suited since their fabrication process would likely introduce simple edge-functionalization in the form of H-atoms or OH-groups, saturating the dangling bonds which resulted from cutting the hexagonal carbon network.

A broad range of computational tools can be used to theoretically determine the dynamical properties, electronic structure, and quantum transport parameters of 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 hydrogen bonds between hydrogenated graphene edges and suitable atomic sites in the nucleotides on the transport properties of this nano-bio system [6,7]. Recently also more ambitious functionalization schemes for graphene edges [8] as well as a promising bilayer graphene setup [9] were investigated by us. Finally, there might be a particular appeal for 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.

[1] R. H. Scheicher, A. Grigoriev & R. Ahuja. DNA sequencing with nanopores from an ab initio perspective. *J. Mater. Sci.* 47, 7439 (2012).

[2] Yuhui He, Makusu Tsutsui, Ralph H. Scheicher, Fan Bai, Masateru Taniguchi & Tomoji Kawai. Thermophoretic Manipulation of DNA Translocation through Nanopores. *ACS Nano* 7, 538 (2013).

[3] Y. He, M. Tsutsui, R. H. Scheicher, C. Fan, M. Taniguchi & T. Kawai. Mechanism of How Salt-Gradient Induced Charges Affect the Translocation of DNA Molecules through a Nanopore. *Biophys. J.* 105, 776 (2013).

[4] H. He, R. H. Scheicher, R. Pandey, A. R. Rocha, S. Sanvito, A. Grigoriev, R. Ahuja & S. P. Karna. Functionalized nanopore-embedded electrodes for rapid DNA sequencing. *J. Phys. Chem. C (Letter)* 112, 3456 (2008).

[5] B. Pathak, H. Löfås, J. Prasongkit, A. Grigoriev, R. Ahuja & R. H. Scheicher. Double-functionalized nanopore-embedded gold electrodes for rapid DNA sequencing. *Appl. Phys. Lett.* 100, 023701 (2012).

[6] Jariyanee Prasongkit, Anton Grigoriev, Biswarup Pathak, Rajeev Ahuja & Ralph H. Scheicher. Transverse Conductance of DNA Nucleotides in a Graphene Nanogap from First Principles. *Nano Lett.* 11, 1941 (2011).

[7] Y. He, R. H. Scheicher, A. Grigoriev, R. Ahuja, S. Long, Z. L. Huo & M. Liu. Enhanced DNA Sequencing Performance Through Edge-Hydrogenation of Graphene Electrodes. *Adv. Funct. Mater.* 21, 2674 (2011).

[8] J. Prasongkit, A. Grigoriev, B. Pathak, R. Ahuja & R. H. Scheicher. Theoretical Study of Electronic Transport through DNA Nucleotides in a Double-Functionalized Graphene Nanogap. *J. Phys. Chem. C* 117, 15421 (2013).

[9] Yuhui He, Makusu Tsutsui, Ralph H. Scheicher, Masateru Taniguchi & Tomoji Kawai. Bilayer Graphene Lateral Contacts for DNA Sequencing. *preprint:* arXiv:1206.4199