# In-silico design of an all-armchair graphene nanoribbon field effect transistor (GNRFET) sensor for the detection of starch

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Starch plays a fundamental role in plants, is an essential molecule to understand energy transport and storage. Therefore, continuous monitoring of intra-cellular synthesis of starch is critical for understanding energy pathways and metabolic regulation in plants. This work highlights the importance of real-time measurement of ultra-low concentration of this metabolite, to detect and manage stress-induced events in plants. Our work presents an in-silico design of an all-armchair graphene nanoribbon field effect transistor (GNRFET) device for the detection of ultra-low concentration (pM-nM) amylose. Starch molecules are composed primarily by two glucose polymers amylopectin and amylose, the later presenting a linear structure desired for its simplicity and smaller size. We use a self-assembled monolayer (SAM) of a pyrene moiety, {3-[4-(pyren-1-yl)butanamido]phenyl}boronic acid adsorbed on the channel, to functionalize the graphene surface. Then covalent binding of the target molecule to the end with phenylboronic acid provides mechanical, chemical and electronic signal sensing stability. Furthermore, we screened configurations with different widths, to control bandgap, lengths to ensure a thermionic transport across the semiconducting junction and different configurations of the back-gated channel in order to optimize electronic transport and switching properties of the device. Our calculations show that the channel functionalization does not affect the electronic signature of the transistor, however further calculations and evaluation with other chemical potentials need to be carried to ensure a clearer measurement of the amylose.

Keywords: field-effect graphene nanoribbon transistor, label-free biomarker sensor, starch nanosensor, amylose nanosensor, phenylboronic acid, pyrene moiety