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POS-D25 – Simulations of DNA-carbon nanotube interactions for the design of field-effect transistors biosensors

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Bioanalytical sensors based on field-effect transistors (bioFETs) are emerging as promising tools to measure the kinetics of biopolymers such as proteins and DNA strands. This class of biosensors is based on an ultra-miniaturized electronic circuit whose conductance is very sensitive to the variations of the electrostatic potential in its environment caused by conformational changes in the biopolymer. Here, we investigate the working of a specific bioFET made of a single carbon nanotube to which is covalently grafted a single DNA strand of the G-quadruplex motif. More specifically, we use advanced sampling techniques based on molecular dynamics simulations to unveil the interactions and kinetics between the biopolymer and the carbon nanotube. We observed that, while the structural stability of the G-quadruplex motif is not significantly altered by the carbon nanotube, some interactions could modify its folding kinetics. We also investigated the origin of the device's sensitivity by characterizing the electrostatic potential around the nanotube as a function of the biopolymer's conformational ensemble. Our conclusions from computational simulations complement the experimental measurements obtained by our collaborators who characterized the same setup. Together, they support the development of this promising biosensor for monitoring the kinetics of biopolymers.

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