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# The electrostatic gating of carbon nanotube field-effect biosensors characterized at the molecular scale using simulations

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Carbon nanotube field-effect biosensors (CNT-bioFETs) are ultraminiaturized devices that can be used to measure single-molecule kinetics of biomolecules. They monitor time scales going from a few microseconds to several minutes, as demonstrated for nucleic acid folding and enzyme function. The sensitivity of CNT-bioFETs originates from the interplay between the nanotube's conductance, which is monitored by the device, and the electrostatic potential generated by the biomolecule under investigation, which is localized on the nanotube. Yet, the origin of this electrostatic gating of the carbon nanotube by a single biomolecule is not well understood at the molecular scale.

To bridge this gap, we employ molecular dynamics (MD) and Hamiltonian replica exchange (HREX) simulations to unveil: (1) the interactions between the biomolecule and the nanotube to which it is attached to the device and (2) the electrostatic potential on the nanotube as the state of the biomolecule changes. We address these questions by considering three prototypical cases: the function of the Lysozyme protein, the hybridization of 10-nt DNA sequence and the folding of a DNA G-quadruplex, which were previously characterized using CNT-bioFETs.

Our simulations show that this protein and these DNAs interact differently with the nanotube to which they are attached. Consequently, the electrostatic potential (ESP) on the nanotube is very sensitive to the type and state of the biomolecule. When compared to experiment, the ESP distribution for the with-ligand and without-ligand states of the Lysozyme protein are in line with the two-level conductance measured by CNT-bioFETs. For the DNAs, however, the ESP distribution for its folded and unfolded states does not agree with the two-level conductance measured. To agree, the DNA strand should not interact with the nanotube, which is not what our simulations suggest. The reason for this apparent conflict could arise from the impact of the external electric field impose by the gate electrode in CNT-bioFETs on highly charged systems such as DNAs, as supported by our recent simulations.

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