SUPPLEMENTAL INFORMATION

Towards quantifying the electrostatic transduction mechanism in carbon nanotube molecular sensors

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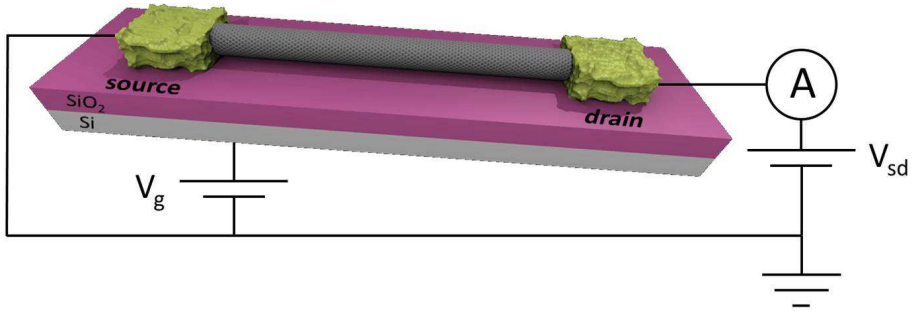
EXPERIMENTAL

Carbon Nanotube Field Effect Transistor. For the experiments in this paper, the carbon nanotube field effect transistor (NT FET) samples consisted of one or a small number of semiconducting NTs, contacted by two electrodes, the source and drain. The carbon nanotube was grown on an oxidized, heavily doped silicon wafer. The bulk of the silicon substrate is highly conducting, so it is able to serve as a gate electrode for the field effect transistor. See the figure for a sample schematic.

Figure S1. Schematic of the NT FET devices used in the experiments described in the main text. A carbon nanotube lies on an oxidized silicon substrate, contacted by source and drain electrodes. The bulk of the substrate is a good conductor that serves as a gate electrode.



Details of the Molecular Dynamics computer simulations. Atomistic molecular dynamics (MD) simulations were performed in order to understand the behavior of each pyrene molecule when adsorbed to CNT. A model for each pyrene molecule was developed according to the AMBER force field[1] protocol. The geometry of each pyrene molecule was optimized with GAUSSIAN[2] using the B3LYP level of theory with the 6-311G* basis set. Partial charges were assigned to each atom using the RESP method.[3] Classical force field parameters were then assigned to the molecule using the general AMBER force field. MD simulations of the pyrene-CNT complexes were performed using the GROMACS[4] MD package. Simulations included explicit water and occurred under ambient pressure and temperature conditions. Simulations of each pyrene-CNT complex were performed with the pyrene adopting a variety of initial configurations. Each simulation was run for about 5 ns in order to sample the preferred dihedral angles of the pyrene functional group when adsorbed to CNT. Trajectories of the simulations were analyzed using VMD.[5]

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