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Silicon nanowire sensor for DNA detection and sequencing: an ab initio simulation WENCHANG LU, YAN LI, MIROSLAV HODAK, ZHONGCAN XIAO, JERRY BERNHOLC, North Carolina State University — Electrical sensors able to detect DNA replication and determine its sequence would enable fast and relatively cheap diagnosis of gene-related vulnerabilities and cancers. At present, it is already possible to electrically monitor DNA replication events using a Klenow fragment of polymerase I attached to a carbon nanotube. Since devices based on Si nanowires would be much easier to produce in quantity, we examine theoretically the sensitivity of a Si nanowire/Klenow fragment for electrical detection of nucleotide addition. A highly parallel real-space multigrid code is used for DFT-based non-equilibrium Green's function calculations involving up to 16,000 atoms, employing highly-accurate variationally-optimized localized orbitals. We find that the open and closed Klenow fragment configurations, prior and during nucleotide addition, respectively, screen the Si nanowire differently and result in a detectable current difference. The sensitivity is the largest in the subthreshold regime while the absolute current difference is maximized in the turn-on state. The sensitivity decreases with an increase of the nanowire size, as expected, but the current difference between different enzymatic states is nearly independent on the nanowire size up to 800 $Å^2$ cross section.

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