

Electrical properties of G4-DNA nanowires

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Understanding the electrical properties of DNA and their derivatives is a necessary step to employ DNA-based systems as active materials for biomolecular nanodevices. However, direct measurements of dc conductivity in DNA-based structures report very contrasting results.

To address such discrepancies we chose well-defined molecular structures, for instance by restricting the base sequence. Among the bases of DNA, guanine (G) is particularly interesting for the possibility to synthesize conductive molecular aggregates, and because of its low ionization potential, which suggests its viability to mediate charge motion along a strand.

By means of first-principle calculations, we investigated the electronic properties of a few guanine solid assemblies: We first studied the electronic structure of pure-model guanine columns, and then we focused on a realistic DNA-derivative (G4-DNA), which consists of a quadruple helix of stacked planar hydrogen-bonded guanine tetramers. We exploit the results obtained from model solid to interpret the peculiar features of the G4-DNA.

We observe that a large π - π coupling may induce a Bloch-like contribution to the conductivity through G stacks, with effective masses similar to those of wide-band-gap semiconductors. The analysis of the electronic structure in G4-DNA shows that, in spite of the localized character of the ground state electron wave functions, the calculated density of states is consistent with a model of a wide bandgap semiconducting nanowire, which hosts effective channels for electron/hole mobility.