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Theoretical study of electron transport in DNA BIKAN TAN, MIROSLAV HODAK, WENCHANG LU, JERRY BERNHOLC, NC State University — Many experiments have observed high conductivity of DNA, but its origin has not yet been satisfactorily explained. In this work, we explore the dynamics of solvated B-DNA sandwiched between metallic nanotubes and connected via alkane linkers. The geometries are relaxed using the CHARMM force field. Conductivities of different snapshots of the system are calculated using the non-equilibrium Green's function method within density-functional theory. Our results show that in certain geometries, the DNA conducts significantly better than in others. For the highest conductivity configuration, a HOMO state extends across DNA's guanine sites to the alkane linkers. In general, we find that the conformational changes strongly affect the energy alignment of HOMO states of the DNA and the linker, and thus have a major effect on the conductivity of the entire system.

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