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Theoretical study of electron transport in DNA BIKAN TAN, MIROSLAV HODAK, WENCHANG LU, JERRY BERNHOLC, CHiPS/NCSU — Multiple experiments have indicated high conductivity of DNA, but its origin has not yet been satisfactorily explained. In this work, we explore the conductivity of double stranded B-DNA using a nonequilibrium Green's function method based on density-functional theory. The DNA is sandwiched between metallic nanotube leads and we investigate the effect of various linkers connecting the DNA to the leads. Our results show that the alkane linker, $(CH_2)_n$, which is often used in experiments, dramatically decreases the conductivity due to its large band gap around the Fermi level. We also find that conductivity can be greatly enhanced by aligning the highest occupied molecule orbital energy of DNA with the Fermi level of the leads by applying a gate bias to the DNA. Finally, we examine the effects of misalignment and mismatches on conductivity of DNA.

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