Modeling charge transport through DNA molecules
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DNA molecule plays an essential role in life phenomenon. As a result of million years of evolution, each half of DNA base pair can recognize its counterpart quickly and accurately. This property provides a great opportunity for building nanostructures in a controllable manner (see e.g., N. C. Seeman, Nature (London) 421, 427 (2003)).

An intriguing question, which has received extensive study, is whether DNA molecule itself is conductive so that one can construct nanowires from DNA molecule. However, existing investigations on this question are somewhat controversial, giving results ranging from insulator, semiconductor, all the way to superconducting (see e.g., R. G. Endres, D. L. Cox, and R. R. P. Singh, Rev. Mod. Phys. 76, 195 (2004)). This can possibly be attributed to the complex chemical property of DNA, the unknown environmental effect, the contact structure, and the charging effect during charge transport.

Because DNA molecules are very complicated, at this moment it is not possible to calculate their charge transport properties by full quantum chemistry methods. The aim of this work is therefore to provide a relatively simple model for investigating transport properties. We take the following strategy. First, we establish a tight binding model which allows us to investigate how various physical factors affect transport in a qualitative fashion. Second, we feed the tight binding model with parameters obtained from an ab initio code so as to include some essential chemical information of DNA molecule.

In the first part of this report, the tight binding model is adopted to simulate a double-stranded poly(G)-poly(C) DNA molecule and analyze general physics of charge conduction. We discuss contact effects due to coupling between the molecule and electrodes; the charging effects due to Coulomb interaction within the molecule; and disorder effects due to randomly distributed ions and twisting distortion. These effects leads to different transport behavior, all of which can be found in the experimental literature.

In the second part of this report, we study a simplified model DNA molecule with density functional theory (DFT): here only the base pairs of DNA are considered. We further assume that the interactions between base pairs are sufficiently weak so that the molecular orbital of each base pair are well-defined. Using Gaussian 98 with B3LYP/6-31G(d), the molecular orbital are computed and couplings between these orbitals are obtained as first order perturbation. In this way, each base pair can be depicted with 9 molecular orbitals, and a few hundreds of parameters are obtained to feed to our tight binding model. Using these parameters, we find that both random sequence and distortion may lead to insulating behavior of DNA, a physics similar to Anderson localization effect in mesoscopic systems.
Molecular Orbitals of G-C pair and A-T pair

Sequence Effect

1  GGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGG
2  AAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAA
3  GCGCGCGCGCGCGCGCGCGCGCGCGCGCGCGCGCGCGCGC
4  ATATATATATATATATATATATATATATATATATATATATAT
5  CGCTTATTTAGTCAAACTAGGCTTAAACGAAATTGTCC
6  CCTAAGATCCTGTGCCCTAGCCGAAGTTAAATCTCGT

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