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Charge Transport in DNA with Five Base Pairs SUNHEE LEE, ERIC HEDIN, YONG JOE, Ball State University — Recently, much interest has arisen in the process of charge transport through DNA due to its fundamental roles in biological processes and in possible novel molecular electronics. We investigate quantum mechanical electron transmission along the long axis of the DNA molecule using a one-dimensional tight-binding model. In this system, we consider a single central conduction channel in which individual sites represent a base-pair formed by either AT (TA) or GC (CG) pairs coupled via hydrogen bonds. The sites are linked by a hopping amplitude, or quantum overlap integral. The sugar-phosphate backbone and the hopping amplitude between each site of the base and the backbone are incorporated into an energy-dependent on-site potential in the main DNA site. For the sake of simplicity, a simple DNA molecule segment with five base pairs is studied, and the transmission for different values of on-site energy is calculated to determine the influence of mismatch (impurity) effects in the DNA sequence. Finally, we present results for the temperature dependence of the transmission, and the current-voltage characteristics in order to examine the extent and efficiency of charge migration. *One of the authors (E.R.H) is partially supported by a grant from the Center for Energy Research, Education, and Service (CERES) at Ball State University.

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