

## **ABSTRACT**

**THESIS:** Charge Transfer through a B-DNA Molecule

**STUDENT:** Dale J Igram

**DEGREE:** Master of Science

**COLLEGE:** Sciences and Humanities

**DATE:** May, 2014

**PAGES:** 92

The interest in charge transport in DNA began in the early 1990s. Since then, numerous publications have experimentally and theoretically provided some insight into the nature of charge migration in DNA. The charge transport properties of DNA have made this molecule very important for use in nanoscale electronics, molecular computing, and biosensoric devices. Early findings have suggested that DNA can behave as a conductor, semiconductor, or an insulator. This variation in electrical behavior is attributed to many factors such as environmental conditions, base sequence, DNA chain length, orientation, temperature, electrode contacts, and fluctuations. To better understand the charge transport characteristics of a DNA molecule, a more thorough comprehension of the electronic coupling and the probabilities of charge transfer between base pairs is required.

To achieve this goal, a mathematical approach for calculating the charge transfer through a DNA molecule has been developed, which utilizes the concepts from Molecular Orbital Theory (MOT) and Electronic Band Structure Theory (EBST). The charge transfer characteristics of the DNA molecule are examined for variation in the twist angle between the base pairs, the

separation between base pairs, and the separation between bases in a given base pair, and will be depicted using 2D graphical representation. By knowing the charge transfer characteristics, the electronic properties (metallic, semi-conducting, insulating) of the DNA molecule can be determined.