# Modeling Charge Transport Through Nucleic Acid Structures

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## Overview

Modeling and simulation of nanostructures is essential in developing new devices. Our group models electron transport in nanoscale devices. We look at charge transport through DNA to study its application as a material for electronic devices as well as possible bio devices for disease detection.

### Motivation

**Sequencing**
Single molecule sequencing

**Bio-Nano technology**
Nano-Sensor

**Charge Transport in DNA**

**Genetics**
Radioactive damages to DNA

**Molecular Electronics**
Molecular wire, tunnel diode

## Model and Method

> **Nucleic acid builder (NAB)** is used for generating coordinates of the atoms.

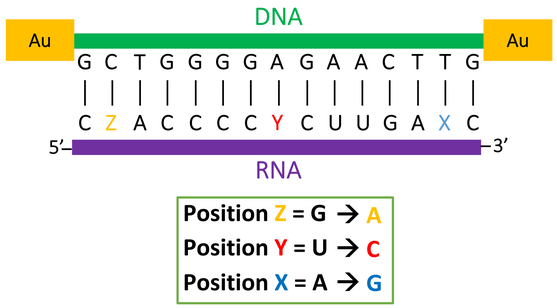
> **Gaussian DFT Package** is used for obtaining Hamiltonian and Overlap matrices.

> **Green's function approach** is used to calculate electron transmission within the **Landauer-Buttiker framework**.

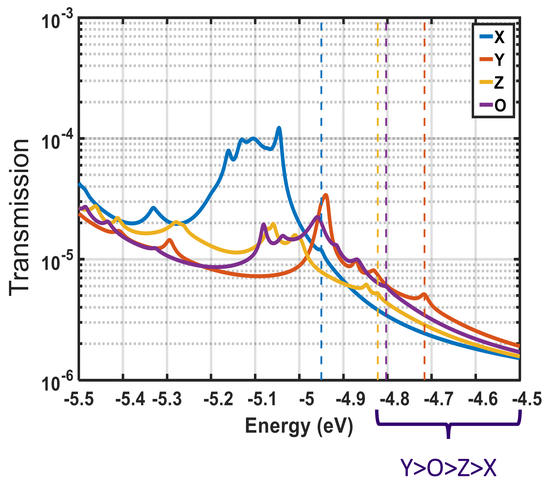
> **Buttiker Probes** are used to capture decoherence.

## Nucleobase Mismatch Detection

> Single nucleobase mismatch detection helps in genetic mutation diagnosis . We test the possibility of using electrical conductance measurements for single mismatch detection in short strands.

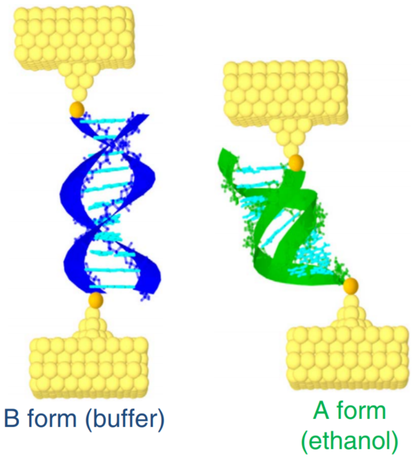


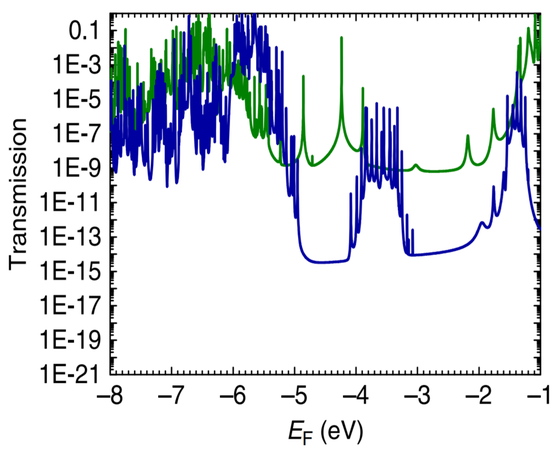

> Mismatches at different locations yield distinct trends for a Fermi energy lying in the highest occupied molecular orbital (HOMO) region.




## DNA Strand as a Switch

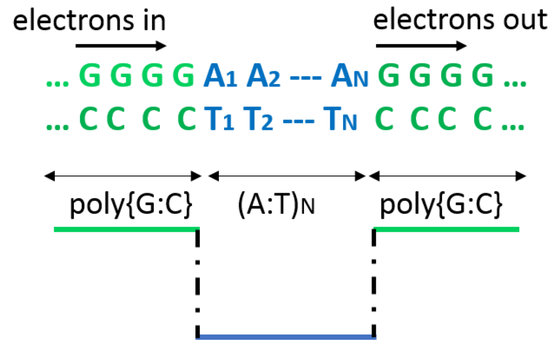
> DNA conformation can be changed by using different solvents. This affects the charge transmission profile of the structure, yielding a switching behavior (high vs low).

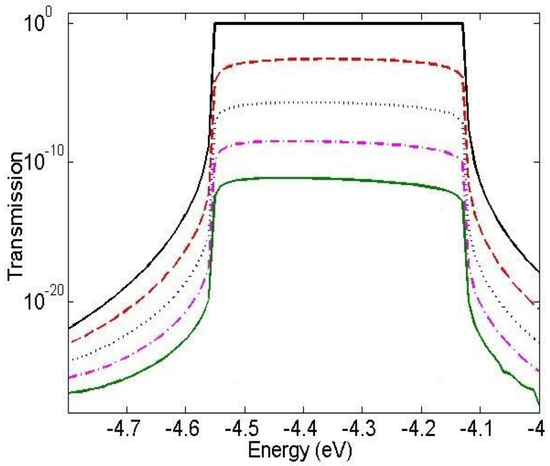



## Tunable Barriers

> Guanine (G) acts as a well and Adenine (A) acts as a barrier for hole transport. As the number of (A) increases, the transmission exponentially decreases.

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## Collaborators

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