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Research Plan

a. Rationale

Single-molecule break junctions are electronic devices which consist of two electrodes separated by a very thin gap in the order of a few nanometers. When the gap is filled by a single molecule, conductance measurements provide insight on the electronic properties of the molecule. Machine learning techniques have recently been developed to separate experimental data from a symmetric single-molecule break junction into different classes, with each class representing a different path for an electron to transport through a molecule. Previous research has not delved deeper into the possibilities of creating mathematical and computational models to represent each of these classes and the aggregate data, taking into account the effects that background tunneling has on measurements taken. I plan to create a computational model to represent any class of data, and the aggregate data, by taking into account the effect of background tunneling. I will create a Python program to find the best fit model for the experimental data in question based on the mathematical model. I also will extract data about the molecule in question, oligo (phenylene ethynylene)dithiol (OPE3), from this model, namely the coupling strengths between channels and electrodes and the channel energy of the molecule. This information about the molecule will later help experimentalists to create more efficient photovoltaic solar cells by isolating which channel is the most efficient for electricity transfer through the molecule.

b. Research questions

The ultimate goal of my research is for my results to be used as foundational knowledge for experimentalists to develop more efficient carbon-based photovoltaics. To gain a better understanding of electron transport through a single molecule break junction, I will create computational models which explain experimental results through a symmetric single-molecule break junction with gold electrodes travelling through oligo(phenylene ethynylene)dithiol

(OPE3). I also will take into account the effects of background tunneling in my model to create a more accurate approximation for the experimental data. To achieve this, the following questions are addressed:

i. How does electric current flow through a single molecule connected between two electrodes?

ii. How can a mathematical and computation model be created to explain conductance histograms for electron transport through single-molecule break junctions?

iii. How does background tunneling affect the shape of a conductance histogram?

c. Methods

i. Procedure

A mechanically-controlled break junction will be used to gather experimental data. Gold electrodes will be split with a gap in the order of a few nanometers, and an oligo(phenylene ethynylene)dithiol (OPE3) will be placed in the gap. There will be a potential difference of 100 mV developed across the break junction. Since single-molecule break junction measurements are intrinsically stochastic, we will require the acquisition of large data sets. We will take approximately 40,000 measurements from the break junction. The break junction will be connected to an ammeter, where current through the molecule can be measured. Knowing the potential difference and the current, we will calculate the resistance. From the resistance, we will calculate the conductance and plot these on a probability density function known as a conductance histogram.

From the existing Landauer-Büttiker Formalism, which establishes the relationship between the transmission probability of an electron given its energy and the coupling strengths and channel energy of the molecule it travels through, generalizations and simplifications can be made to create a model that applies to a symmetric non-resonant break junction. We will assume that the coupling strength and channel energy of the molecule are independent random variables that are normally distributed. We also will assume that the height and spatial width of the energy barrier to tunneling are distributed uniformly and log-normally, respectively. We will combine

two separate models for non-resonant electron transport and background tunneling to create a model for the flow of electrons that fits all classes of data for any molecule.

ii. Risk and Safety Analysis

1. Human Subjects: N/A
2. Vertebrate Animals: N/A
3. Potentially Hazardous Biological Agents (PHBA): N/A
4. Hazardous Chemicals/Activities/Devices: N/A

iii. Data Analysis

The data obtained from experimental means will be separated into different classes using machine learning techniques, which each represent a different path for an electron to travel throughout the molecule. Class 1 will represent transport through background tunneling which occurs even though a molecule still fills the gap, class 2 will represent single-molecule transport through the benzene rings of OPE3, and class 3 will represent single molecule transport through the gold-sulfur bonds of OPE3. A mathematical model will be created which takes into account background tunneling and uses constant values for the coupling strength to the electrodes and the channel energy of the molecule to predict the conductance of the molecule. I will create a Python program that, using guesses for the constant values, will create the best fit model for the experimental data. The coupling strength and channel energy of the molecule, as well as the conductance peak of the molecule are of special interest to experimentalists, as these values will allow them to create more efficient solar cells.

d. Bibliography

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[5] Williams, Patrick D., and Matthew G. Reuter. "Level Alignments and Coupling Strengths in Conductance Histograms: The Information Content of a Single Channel Peak." The Journal of Physical Chemistry C, vol. 117, no. 11, 12 Mar. 2013, pp. 5937–5942., doi:10.1021/jp310180s.

1. **Human participants research:**

   N/A

2. **Vertebrate animal research:**

   N/A

3. **Potentially hazardous biological agents research:**

   N/A

4. **Hazardous chemicals, activities, and devices:**

   N/A

No Addendums EXIST