OFFICIAL ABSTRACT and CERTIFICATION

Modeling the Conductance of Single-Molecule Electron Transport in a Symmetric Break Junction

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A break junction is an electronic device that consists of two electrodes separated by a very thin gap in the order of a few nanometers. Electron transport through an Oligo(phenylene ethynylene)dithiol (OPE3) molecule in a mechanically-controlled break junction with gold electrodes through a potential difference of 100 mV was measured with 41916 trials. The data was separated into 3 classes corresponding to different channels through which electrons could flow. Class 1 represented quantum tunneling through the electrodes, Class 2 represented single-molecule transport through the benzene rings of the OPE3 molecule, and Class 3 represented single-molecule transport through Au-S bonds in the molecule. A probability density function was constructed to model non-resonant symmetric tunneling based on the assumption that coupling strengths between the channels and electrodes, as well as the channel energies, are normally distributed. A Python program was developed to find the best fit line for the experimental data collected from the OPE3 molecule. Molecule's channel energy and coupling strengths were extracted from the model. All prominent channels are well-described by the model, and the inclusion of the background tunneling is necessary to eliminate a fitting error of approximately 25%. OPE3 is used in polymer form in carbon-based photovoltaics, so understanding how electrons flow through the molecule is critical in designing more efficient solar cells.

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