

Brief Report

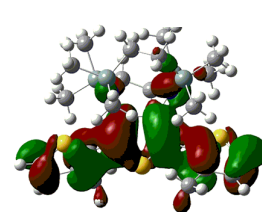
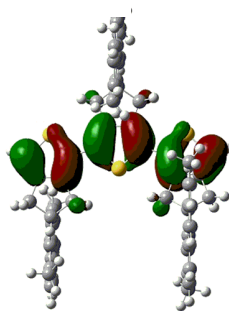
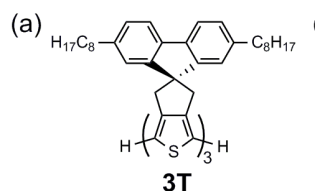
Lee See Kei

11.02.22

Experiment Work

Part 1: Break Junction Testing

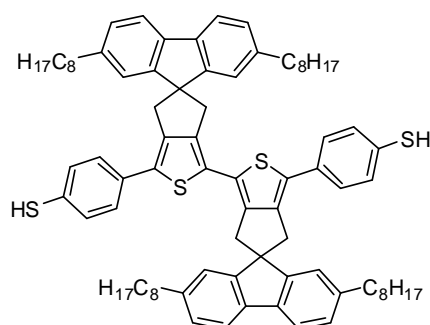
New molecules from Ie-sensei at room temperature (RT)



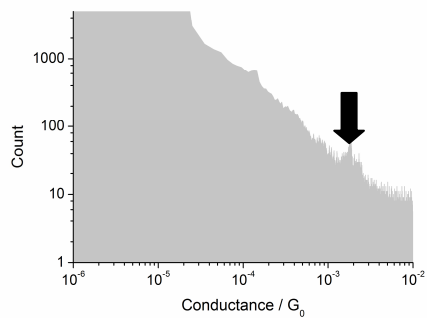
Chemical structure and HOMO of (a) molecule 1 and (b) molecule 2

- HOMO of molecule 1 is delocalized over the whole p conjugated backbone, which is a typical characteristic of non-substituted oligothiophenes if compared to molecule 2 due to its planar/flat structure.
- Expectation: Conductance value for molecule 1 should be better than molecule 2.
Note: Anchoring groups for both molecules are different. However, it won't affect the distribution of the electrons.

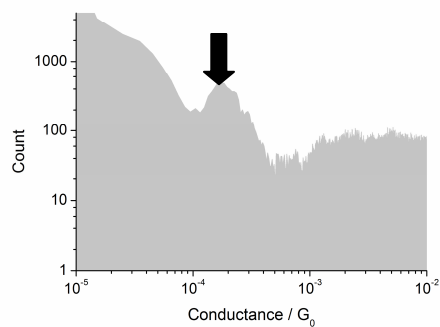
The structure of the simplest molecule, HS-2T-SH is shown as follows.



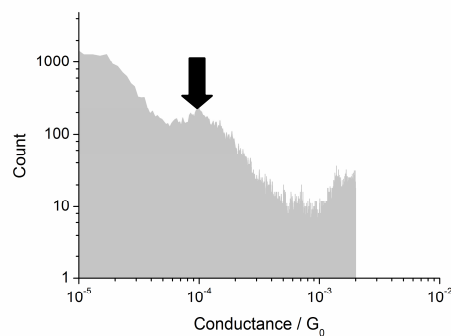
Break-junction testing was performed to determine the conductance of this new molecule and the following results were obtained:



2T (1.86 nm)



4T (2.64 nm)



6T (3.61 nm)

Based on the results, we can observe that as the molecular length increases, the conductance values decreased.

Part 2: Thermoelectricity

It had been suggested that the value of S can indicate the sign of the charge carrier and the relative position of E_F with respect to HOMO / LUMO levels. Thus, I am interested to determine the Seebeck coefficient, S .

Things to do:

- Prepare measuring device and related software
- Learn how to conduct thermoelectric measurements
- To test whether the system is working fine.

Compare with the results obtained by Segalman's group (To try it out with the molecule – benzenedithiol)