

Supplementary materials

February 5, 2024

1 Current of the ben-ant model with thiol

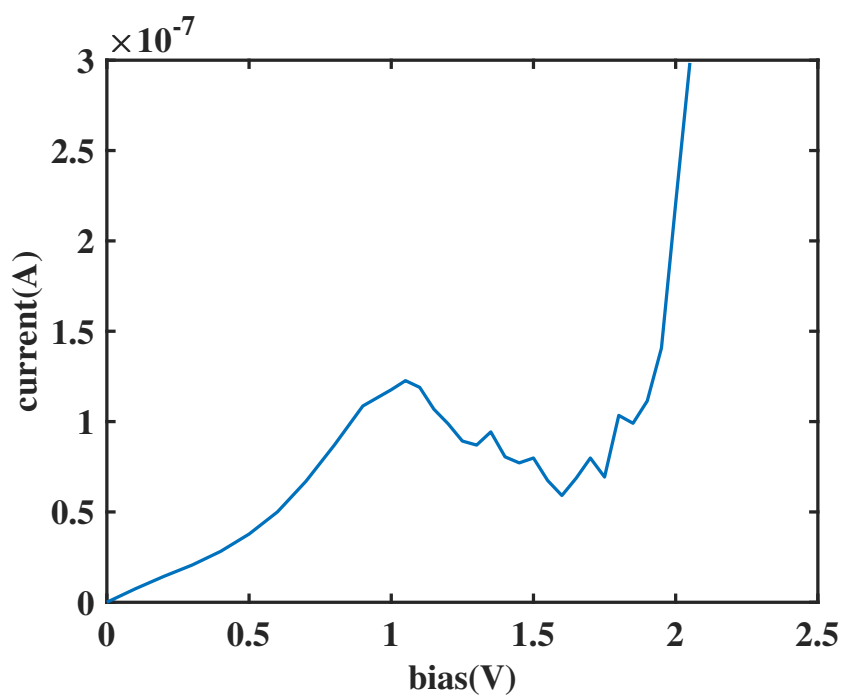


Figure 1: The I(V) figure of the ben-ant-S model

2 Pdos of the ben-ben models with additional functional groups

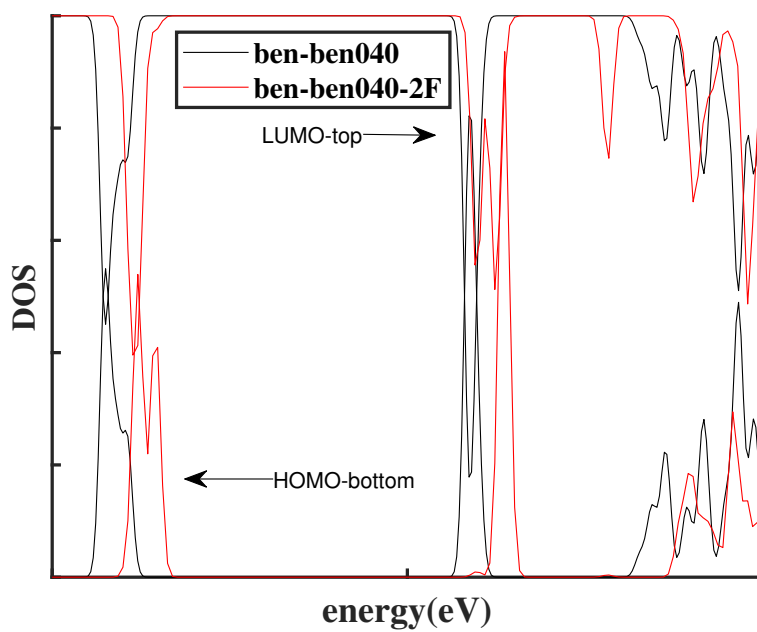


Figure 2: The pdos figure of modified ben-ben040. Black: original ben-ben040
 Red: ben-ben040-2F. We have aligned the vacuum level energy of these two molecules. The orbitals that we determine the $HOMO_{bottom}-LUMO_{top}$ gap are labelled as HOMO-bottom and LUMO-top

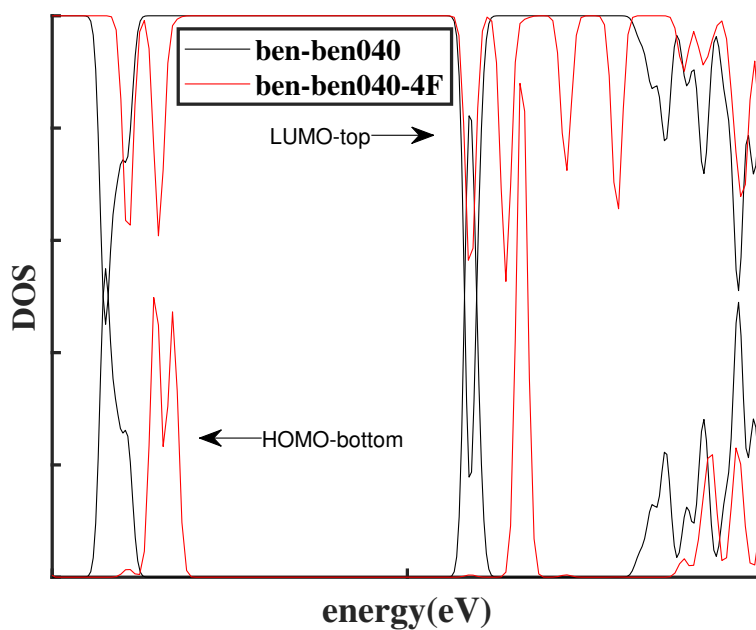


Figure 3: The pdos figure of modified ben-ben040. Black: original ben-ben040
 Red: ben-ben040-4F. We have aligned the vacuum level energy of these two molecules. The orbitals that we determine the $HOMO_{bottom}-LUMO_{top}$ gap are labelled as HOMO-bottom and LUMO-top

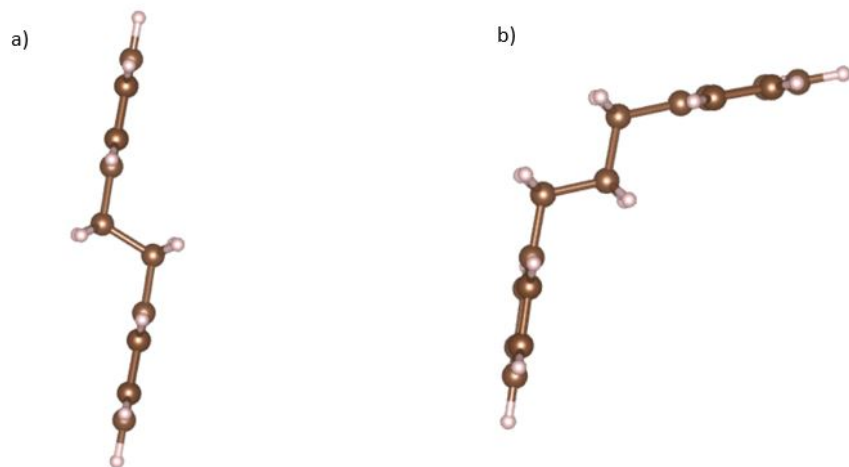


Figure 4: The geometry of a) ben-ben020 b)ben-ben030 the geometries of the models with an even number of CH₂ groups are different to those with an odd number of CH₂ groups. Different geometries affect electron transport, therefore we would not expect a linear relation between reduction of current and chain length.

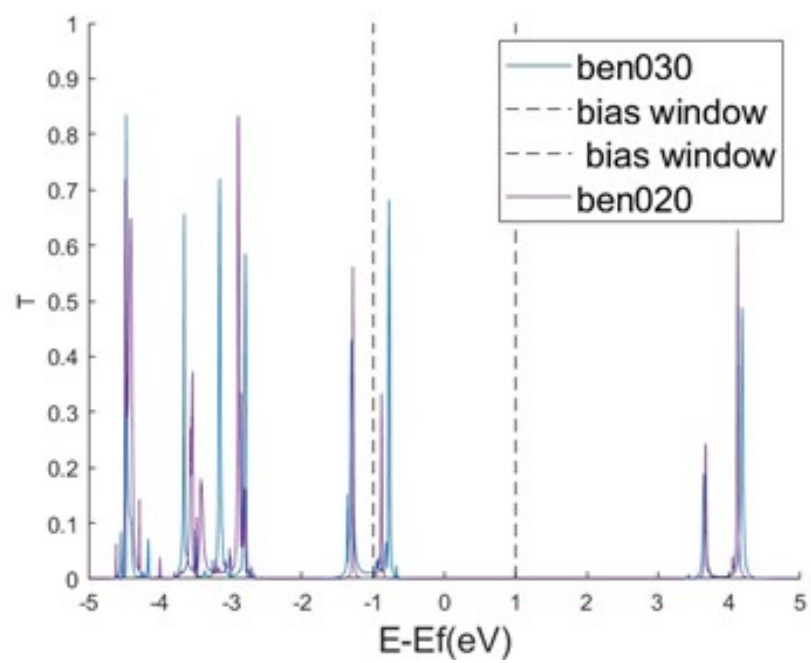


Figure 5: The transmission plot of ben-ben020 and ben-ben030. Within the bias window the transmission peak for the ben-ben030 molecule is larger than that of ben-ben020. The larger transmission peak in ben-ben030 correlates with greater electron flow at the same bias, resulting in a higher current.