Engineering Transport Orbitals in Single Molecule Junctions

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Single-molecule devices provide an ideal platform to study quantum transport for a new generation of electronic components, as molecular design enables the integration of electronic functions at the smallest level [1]. Charge transport can be tuned using electron-donating substituents, just like traditional semiconductors [2]. In this work, single-molecule devices based on compounds in Figure 1a, including either electron withdrawing or donating side groups into a tolane molecular structure, are fabricated and characterized using the STM-break junction technique at ambient conditions. Measuring the electrical conductance and the thermopower we find that the electron withdrawing side groups can be used to tune the energy levels of transport orbitals and create additional charge transport channels due to quantum interference effects for the enhancement of charge transport properties.

Figures

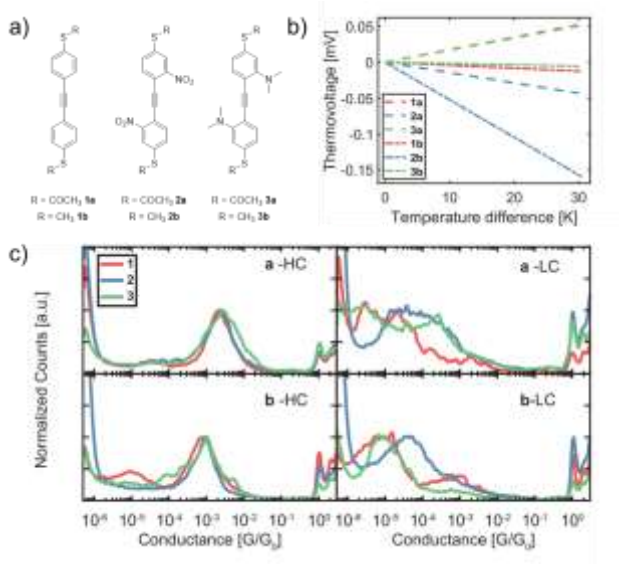

Figure 1: (a) Schematic view of tolane **1** with either electron withdrawing **2** or donating **3** side groups, decorated with either –SAc **a** or –SMe **b** anchor groups. (b) Linear fit of all the temperature difference dependent thermovoltage values for all the compounds to obtain the themopower, combined for comparison. (c) 1D-conductance histograms of the HC (left) and LC (right) peaks as obtained from clustering, separated by anchoring group (top: -SAc, bottom: -SMe). Measurements have been normalized by peak height to make the peak position and shape directly comparable across the different molecules

References

[1] D. Xiang et al., Chem. Rev. Lett., 116 (2016) 4318
[2] L. Venkataraman et al., Nano Lett., 7 (2007) 502
[3] A. Daaoub et al., J. Phys. Chem. Lett., 13 (2022) 9156