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Quantum Interference-Induced Conductancce Variation in Mechanosensitive Single-Molecule Junction

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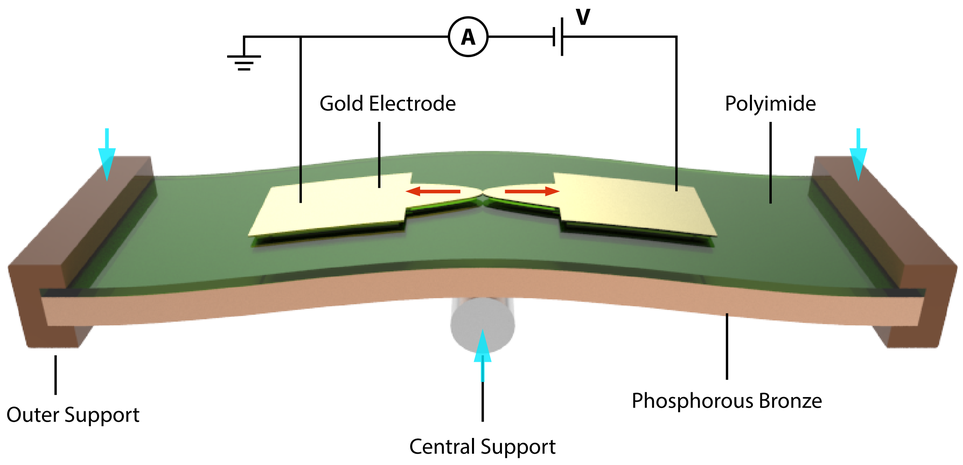
Mechanically-Controlled Break Junction

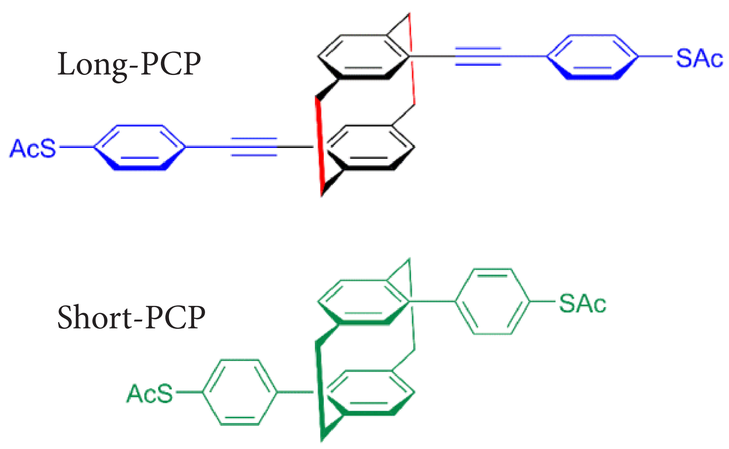
- Atomically-sharp electrodes are formed by the mechanical stretching of the gold wires, where quantized conductance can be observed[1].
- This atomic-sized contact grants a good platform for single-molecule study.
- The mechanically stretching can be controlled with sub-nanometer resolution and allows large statistics in molecular measurement.
- Mechanical strain can be introduced to the molecule via bending.

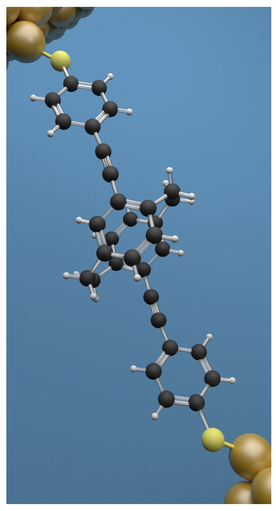


1. Agraït, N., Yeyati, A. L. & van Ruitenbeek, J. M. Quantum properties of atomic-sized conductors. Phys. Rep. 377, 81–279 (2003).

Cyclophane-based Mechanosensitive Molecules

- Cyclophane-based molecules: π-stacking system with covalent bond
- Flexible cyclophane can be subjected to strain and compression, which can introduce modifications in the molecular orbital. This can lead to a change in the electronic transmission through the molecular junction.

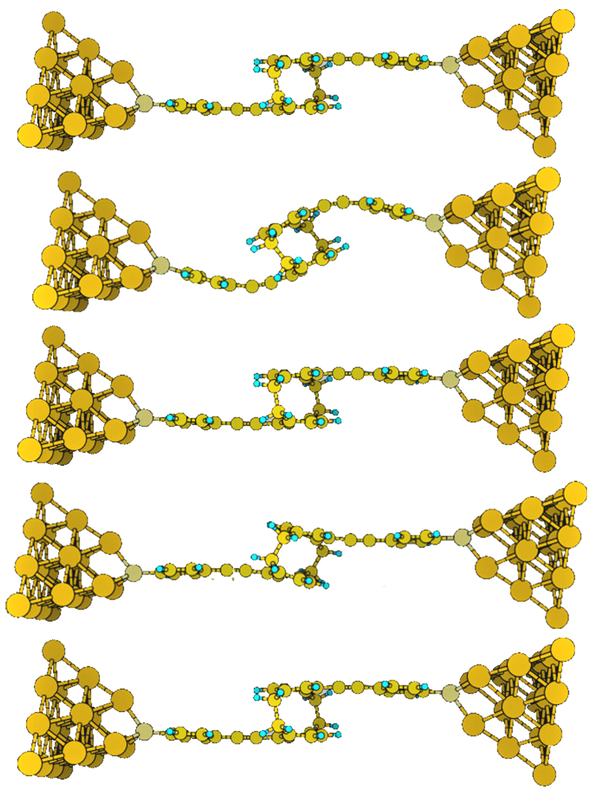




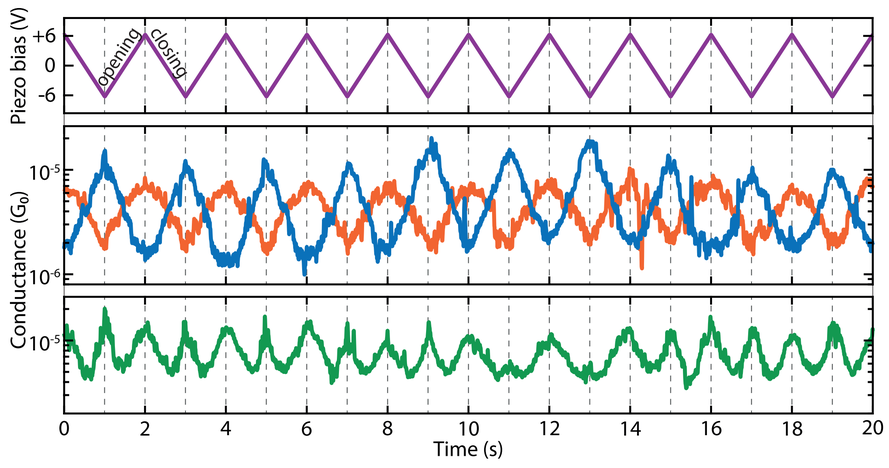
Cyclophane-based moelcules (PCP) studied in MCBJ. (Sythesized by Mayor group, Basel)

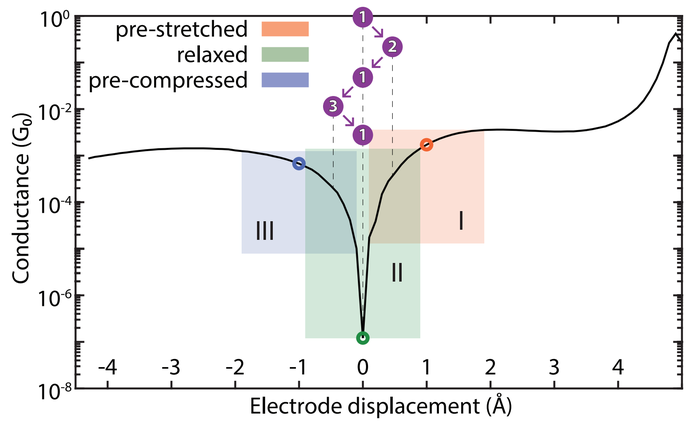
Quantum Interference-Induced Conductance Variation

Long-PCP



- In the conductance modulation experiment, a piezoelectric stack modulates the electrode displacement of the molecular junction. This can induce compression and stretching of the PCP molecule.
- As the electrode opens and closes, we observe 3 scenarios where the first 2, conductance either goes up and down in/out-phase compared to the electrode movement. In the third case, a double frequency of the conductance modulation is observed.
- This, according to DFT calcuation, can be seen as a result of destructive quantum intereference. In the case of double frequency, the molecule change its conductance across the interference dip, while the other cases, the molecule changes its conductance only around the dip[2].
- Similar conductance variation has also been observed in the Short-PCP molecule, which is likely due to the same mechanism.



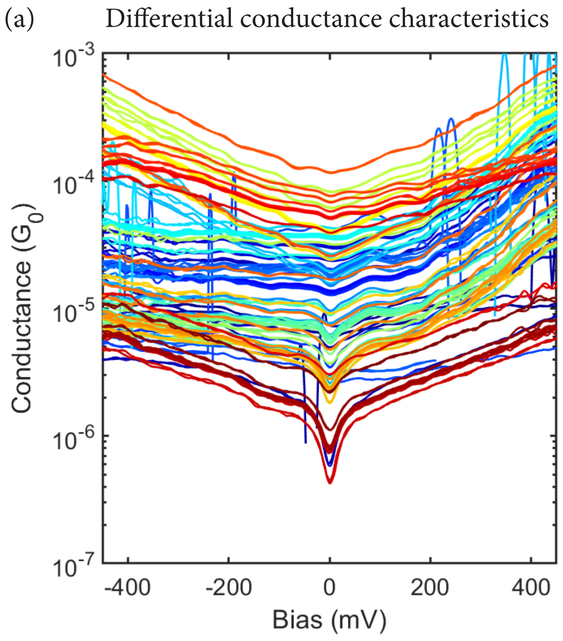


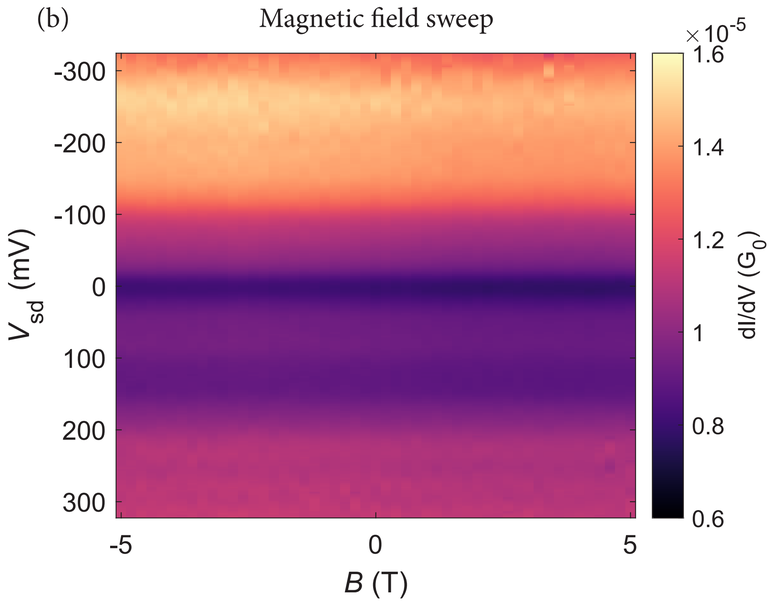
2. Stefani, D. et al. Large Conductance Variations in a Mechanosensitive Single-Molecule Junction. Nano Lett. 18, 5981–5988 (2018).

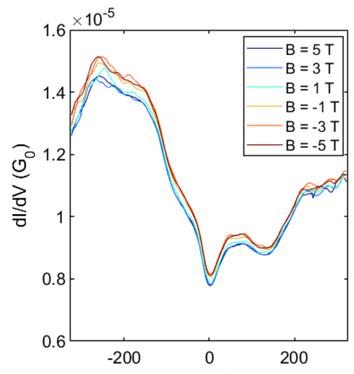
Short-PCP

- To study the detailed electronic transmission of the PCP molecules and corresponding quantum intereference properties, IV characterizations on the Short-PCP were performed at 4.2K.
- In (a), we modulated the electrode displacement and measured a large variation of conductance values. Particularly, a dip close to zero bias at low conductance value is consistently observed. The origin of this unique feature is under investigation.
- In addition, differential conductance is also measured as function of magnetic field. Interestingly, the features are independent of the magnetic field applied, which suggests that they are not from phase-coherent process in the gold electrodes.

Low Temperature IV Characterization







Cross section of differential conductance in magnetic field sweep: The dip position is independent of the magnetic field applied.

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