Conductance of 4,4’-Bipyridine Single-Molecule Junctions with Silver Electrodes

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Introduction

Metal-molecule surfaces in single-molecule junctions effectively influence conductance, the most fundamental transport property.[1] Gold (Au) is the most commonly used electrode material due to its chemical inertness.[2] However, other metals, like silver (Ag), are seldom used due to their instability and tendency to oxidize.[4] In this study, we employ a modified Scanning Tunneling Microscope-based Break-Junction (STM-BJ) setup inside a glove box to measure the conductance of 4,4’-Bipyridine (BP) single-molecule junctions with Ag and Au electrodes in N_2.

Methods

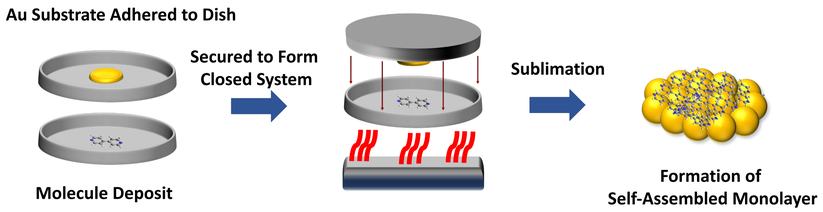

Figure 1. 4,4’-Bipyridine molecules are deposited onto Au substrates via sublimation

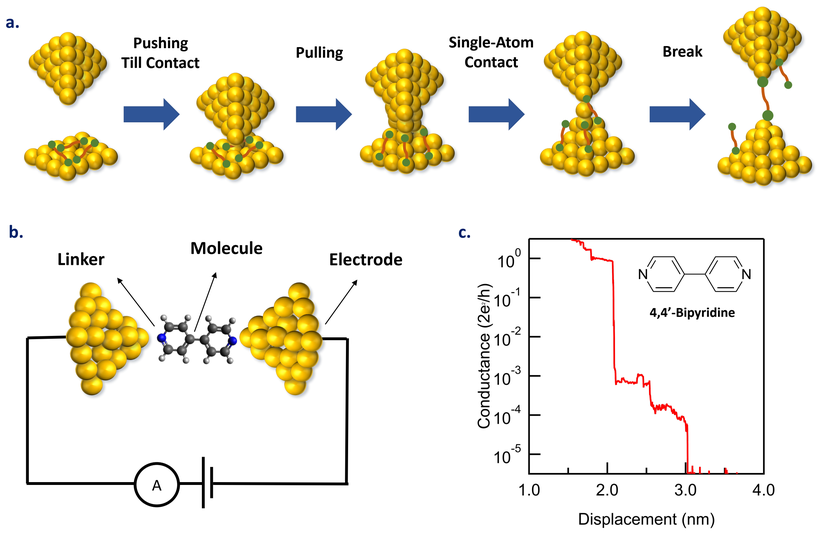

Figure 2. (a) Formation of molecular junction upon contact with a SAM **(b)** Scheme of STM-BJ circuit **(c)** Sample trace of conductance versus displacement for Au electrodes

STM-BJ Results

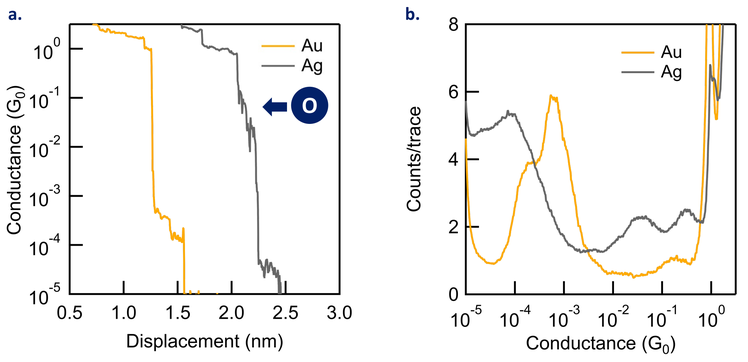

Figure 3. (a) Sample conductance traces and **(b)** logarithmically binned conductance 1D histograms (4000+ traces compiled without data selection)for BP measured with Au and Ag electrodes.

- Ag-tip BP junctions exhibit lower conductance compared to Au-tip junctions
- Ag-tip BP junctions display a single conductance peak, while Au-tip junctions have a double conductance feature
- There are features indicating the formation of Ag-O-Ag junctions at conductance's higher than $10^{-2}G_0$

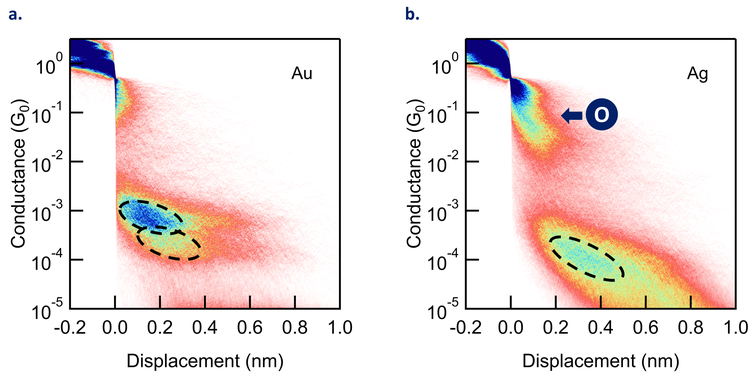

Figure 4. 2D conductance histograms measured with Au **(a)** and and Ag **(b)** tips. Dashed lines are indicative of junction geometries.

- Au electrodes display two regions, attributed to specific junction geometries
- Ag electrodes exhibit a distinct absence of the double peak feature across a wider range of displacement lengths, concurrently resulting in hindered lower conductance values
- Notably, Ag-O-Ag junctions can be observed at ~ 0.1 nm

Junction Geometries

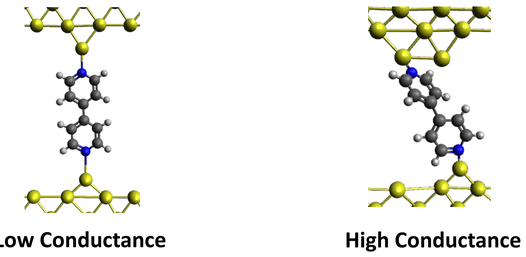

Figure 5. Potential Junction Geometries for BP measured with Au electrodes

- Ag can inhibit all potential geometries found in Au, but due to reduced van der Waals interactions, only 1 peak is apparent.[3]

Conclusions

We measured the conductance of BP molecular junctions using STM-BJ technique with Au and Ag electrodes. Experimentally, we find lower conductance in Ag-tip junctions compared to Au, which could be attributed to the lower coupling strength at the Ag-molecule interface. Furthermore, Ag-tip junctions lack the characteristic double peak feature observed in Au due to reduced van der Waals interactions. Formation of Ag-O-Ag junctions indicate that our protocol for creating these junctions in a glove box is not yet optimized. In the future, theoretical studies should be conducted to further understand these results.

Acknowledgements

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