Quantum interference in molecular junctions

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In mesoscopic structures, such as Aharanov-Bohm rings, destructive (constructive) electron interference leads to a decrease (increase) in sample conductance. Molecules are perfect candidates to study similar quantum effects at higher temperatures, since their energy level spacing is large ($\sim$ eV). Specifically, for junctions containing cross-conjugated molecules, destructive interference is anticipated at certain electron energies. Here, we report direct evidence for interference effects in molecular junctions at room temperature. For this, we first synthesized a family of (di)thiolated organic molecules. The molecules are different in their central ring only, but have different conjugation nevertheless (cross-conjugation vs. linear conjugation). Subsequently, the molecules were self-assembled in a compact monolayer (SAM) on a gold-coated Si-substrate. Charge transport measurements were done by making use of conductive atomic force microscopy (c-AFM). Our results show a profound difference between the cross-conjugated anthraquinone derivatives and the linearly conjugated molecules, both in conductance values and in actual dI/dV-curves. Moreover, our data for the cross-conjugated molecules are fully consistent with destructive interference via orbital pathways, as confirmed by extensive transport calculations (DFT+Σ-approach). All in all, our study demonstrates a fundamentally new quantum phenomenon in molecular charge transport. Moreover, it opens the road for a new type of molecular switches. These could be based on either chemical or electrostatic control of quantum interference.