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“Apparent reversal of the order of particle-in-a-box-like states in a single molecular wire”
Part I

Abstract:

For the use of single molecules as devices, engineering and control of their electronic properties is important. Most intriguing in this respect are electron correlation effects, which are intrinsically strong in molecules due to their small size. Among these, Coulomb charging energies play a most important role. Coulomb charging energies strongly depend on the localization of electrons and hence on the localization of the orbitals they occupy. It is therefore not surprising that the orbital sequence of a given molecule can reverse upon electron attachment or removal, if some of the frontier orbitals are strongly localized while other are not. However, in molecular wires, only those orbitals delocalized over the entire molecule dominate the conductance, and hence to implement functionality therein, a control of these orbitals is desired.

From a set of scanning tunneling microscopy (STM) and spectroscopy (STS) measurements, we will show that the orbital sequence in a single molecular wire of individual dicyanovinyl-substituted quinque thiophene (DCV5T) on ultrathin insulating films can be engineered to achieve near-degeneracy of the two lowest lying unoccupied molecular orbitals. These orbitals visualized directly in real space are the lowest two of a set of particle-in-a-box-like states and differ only by one additional nodal plane across the center of the wire. Upon charging, the sequence of these two orbitals is apparently reversed and the state with one more nodal plane is imaged at lower bias.