Contacting Single Molecules With The STM: Model Systems For Molecular Electronics

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Molecular electronics is a promising field for future applications as single functionalized molecules can be used as devices that perform the basic functions of digital electronics [1]. A simple system is that of a molecular wire, which should enable a controlled maximum charge transport. The configuration of such a wire, in contact with a metallic electrode, plays an important role. Ideally, it should be in a planar geometry and decoupled from the substrate (Fig.1). So-called Lander molecules are very suitable in this regard, because they are equipped with spacer legs. The electron transport through the contact between the molecule and a metallic electrode plays a crucial role in the quality of a molecular device, because any functionalized molecular unit in a device must be electrically contacted to other units or to electrodes.

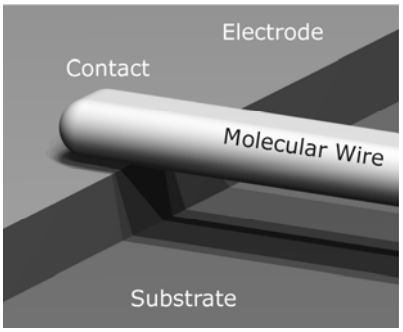

Figure 1: Scheme of a molecular wire – electrode junction.

Manipulation of single molecules with the scanning tunneling microscope (STM) at low temperatures allows to bring molecules in desired positions and conformations, which are not present directly after deposition. Several examples of molecular wire – electrode systems will be presented, where single molecules are contacted by STM in a controlled way. Different molecules of the Lander family have been contacted to step edges on a Cu(111) surface [2] and to characteristic nanostructures on Cu(110) [3,4]. These nanostructures, formed by the molecules themselves, act as contacting pads for the molecular wire with suitable dimensions, having a width comparable to the width of the wire. The changed chemical structures of the molecule and on the other hand different shapes and dimensions of electrodes lead to a variety of contact configurations.

The molecule-electrode contact is characterized by the additional contribution to the tunneling current in the STM image, but also by the influence on the electronic states of the electrode. An important parameter for the charge transport through the junction is the vertical distance between the molecular wire and the metal atoms of the electrode. The quality of the contact is discussed by means of this distance and of the chemical composition of the molecular end group. Experimental results are compared with calculations.

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