

Assembly of surface-supported metallic quantum wires and their interaction with single organic molecules

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Low-temperature scanning tunneling microscopy/spectroscopy (LT-STM/STS) provides an ideal experimental tool to study low-dimensional electron systems since it enables both the characterization and manipulation of single molecules and atomic-scale structures at surfaces [1]. Assembled structures of special interest in terms of ultimate miniaturization are atomic chains serving as *quantum wires* which will play a leading role in future nanoscale electronics. We have employed LT-STM/STS to assemble monatomic Cu chains on Cu(111) by atomic manipulation at 7 K, to explore their electronic structure, and to study their interaction with single pentacene molecules (pentacene is a linear hydrocarbon consisting of five benzene rings). Spectroscopic measurements of the differential conductance [as a measure of the local density of states (LDOS)] reveal that the bare Cu/Cu(111) chain exhibits quantized onedimensional (1D) electronic states trapped in the pseudogap of the projected Cu bulk bands [2]. In detail, the Cu/Cu(111) monomer is associated with a sharp quasi-atomic resonance at 3.3 eV above the Fermi level. For assembled Cu chains, the coupling between these resonances yields a series of bound chain-localized states. The square of the corresponding wavefunctions can be determined by measuring the spatial variation of the dI/dV signal at tunneling voltages where peaks in the LDOS are observed. The resulting dI/dV maps (cf. Fig. 1) reveal clear symmetry properties of the corresponding eigenstates indicative for quantum confinement in a 1D potential well. The $E(k)$ dispersion of these states is fully described by an effective 1D tight-binding Hamiltonian (cf. Fig. 2).

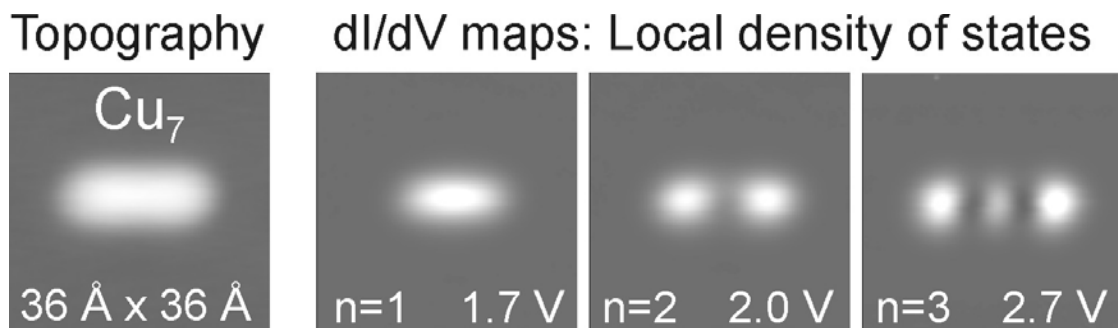


Fig. 1 Left: Constant-current image (1 nA, 1 V, $36 \text{ \AA} \times 36 \text{ \AA}$) of a Cu_7 chain (Cu-Cu spacing 2.55 \AA) oriented along the close-packed rows of the Cu(111) substrate. Right: dI/dV maps measured at constant tip height for different voltages showing the spatial distribution of the LDOS with n denoting the number of lobes of the wavefunction.

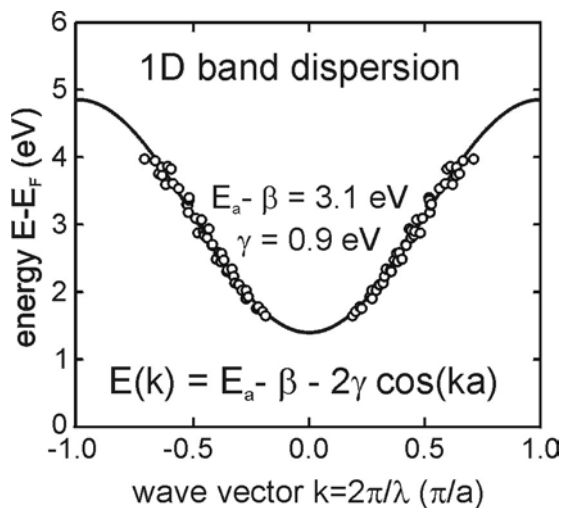


Fig. 2. 1D band dispersion extracted from the characteristic wavelength for chain lengths from 5 to 15 atoms and $n=3$ to $n=8$. The wave vector is given in units of π/a ($a=2.55$ Å is the Cu-Cu spacing). The experimental data are well fitted within the tight-binding approximation yielding a band centered at 3.1 eV and a band width of 3.6 eV (equivalent to an effective electron mass of $m^*=0.68m_e$).

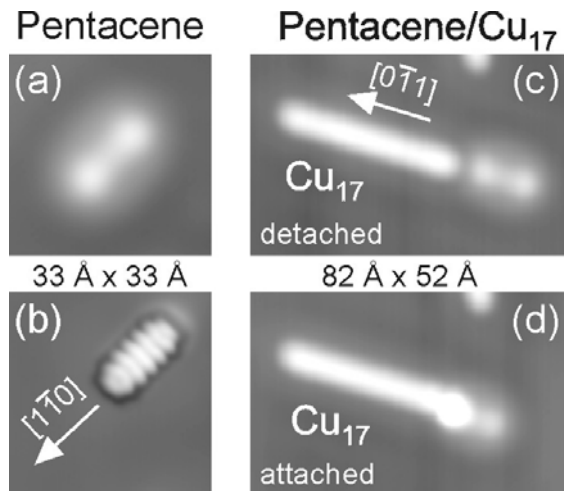


Fig. 3. Pentacene molecule imaged (a) with a bare metallic STM tip and (b) probed with submolecular resolution after transferring a molecule to the tip prior to imaging. The molecules adsorb in a flat geometry with their long axis parallel to the close-packed Cu rows of the substrate. Panels (c) and (d) show a Cu_{17} chain and a pentacene molecule (c) before and (d) after attachment by lateral manipulation.

The present finding of quantum wire behavior in a metallic one-component system is of considerable importance since it avoids the structural and electronic complications inherent to heterogeneous systems and thus provides an ideal 1D electronic model system. Taking advantage of this circumstance, we have addressed the contacting of single pentacene molecules to these model quantum wires. Our measurements reveal that (i) lateral manipulation allows to connect single molecules to the chain ends in a well-defined way [cf. Figs. 3 (c,d)] and that (ii) the molecule/chain interaction shifts the 1D quantum levels of the monatomic Cu wire to higher binding energies. We stress that the present system represents an instructive model case to study the implications of single molecule contacting by metallic nanostructures. A detailed understanding of this fundamental process is of central importance in order to push forward the frontiers towards lateral networking of functional molecules on an atomic level.

[1] See e.g.: D. M. Eigler and E. K. Schweizer, *Nature (London)* **344**, 524 (1990); G. Meyer, S. Zöphel, and K. H. Rieder, *Phys. Rev. Lett.* **77**, 2113 (1996).

[2] S. Fölsch, P. Hyldgaard, R. Koch, and K.H. Ploog, *Phys. Rev. Lett.* **92**, 56803 (2004).