# Atomic scale structure, electronic and vibrational properties of one-dimensional *sp-sp²* carbon-based nanostructures

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Hybrid *sp-sp²* carbon-based nanostructures have recently attracted interest due to the possibility to form novel organic systems, such as one-dimensional (1D) carbon atom wires [1], with tunable electronic and optical properties for a wide range of potential applications. Raman spectroscopy is known to be a powerful technique to characterize the vibrational properties of low-dimensional carbon materials, providing valuable information on structural properties and hybridization states of carbon atoms [2]. More recently, surface science investigations have shown the possibility to synthesize *sp-sp²* carbon nanostructures on metal surfaces and observe them *in situ* at the nanoscale by scanning tunneling microscopy (STM) [3][4].

In this work, aiming to exploit the potentialities of the aforementioned experimental approaches, we combine *in situ* STM and Raman spectroscopy to investigate the morphological, structural, electronic and vibrational properties of 1D *sp-sp²* carbon structures synthesized on Au(111). The molecular precursor, which is a linear molecule where two inter-connected phenyl groups are terminated at each end by Br atoms, is evaporated onto the Au substrate, kept at room temperature. This procedure results in the on-surface synthesis of linear structures, as revealed by high-resolution STM imaging (fig. 1). Surface Au atoms are likely to play a key role in the synthesis mechanism, catalysing the dehalogenative coupling between the precursor molecules. Post-deposition annealing at temperatures around 400 K induces a more disordered arrangement of molecular chains, possibly caused by the thermal activation of surface diffusion. To study the electronic properties, we performed scanning tunneling spectroscopy (STS) measurements and Density Functional Theory (DFT) calculations of the electronic structure. These calculations also allow the simulation of STM images, supporting the interpretation of experimental data. Raman spectroscopy, performed *ex situ*, reveals the characteristic vibrational features of *sp*- and *sp²*-hybridized carbon around 2200 $cm^{-1}$ and 1600 $cm^{-1}$, respectively (fig. 2), thus providing unambiguous evidence of the formation of hybrid *sp-sp²* carbon nanostructures. The interpretation of Raman spectra is also supported by first-principles calculations of the vibrational properties of the system.

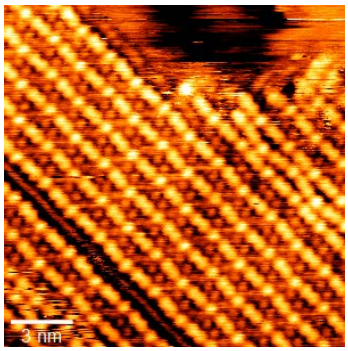


*Figure 1: High-resolution STM image of 1D sp-sp² carbon chains synthesized on Au(111) at room temperature.*

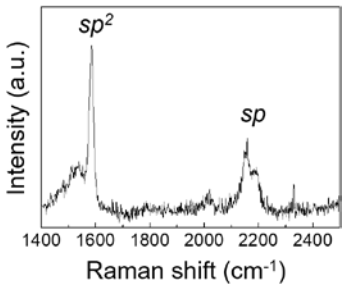


*Figure 2: Raman spectrum of 1D sp-sp² carbon chains.*

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