Local effects on inelastic electron tunneling spectroscopy at single molecular junction

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Charge transport through metal-molecule systems is a major subject of study in a rapidly growing interdisciplinary research field. It deals with fundamental and applied aspects of science at the nanoscale aiming to control the electron conductance at the molecular level and the uprising of nanotechnology. One of the major results of this research is that the properties of an isolated molecule are not the only fundamental parameters determining the conductance in a metal-molecule junction. Indeed, similarly to the adsorption of molecules on surfaces, the atomistic arrangement at the junction and the coupling between the molecule and the metal electrodes can significantly alter the electronic and structural properties of the molecule. It is therefore important to characterize the metal, molecule and the metal-molecule system to identify the factors which influence the electron transport.

At this aim a scanning tunneling microscope (STM) at low temperature has been applied to measure the transport properties of single molecules supported on metal surfaces. This microscope allows characterizing the transport properties as a function of tip-sample distance which can vary progressively from tunneling to point contact regime. Specifically, the molecular vibrations, which reflect the molecule-metal coupling, have been characterized from tunneling up to the formation of the contact. As the transport properties can strongly depend on the properties of the contacting electrode, the vibration spectrum of the tip has been measured to determine the atomistic structure of the tip apex [1]. Given the atomistic structure of this, the vibration modes of an isolated carbon monoxide molecule adsorbed on Cu(111) has been monitored as a function of distance from a copper electrode [2]. A continuous blue shift of the frustrated rotation mode in tunneling followed by an abrupt softening upon the contact formation was observed. This indicates that the presence of the metal electrode sensibly alters the structure and conductive properties of the junction even without the formation of a strong chemical bond.

Finally, I will show that inelastic tunneling electron can trigger the formation of a transitory metal-ligand bond between a copper atom and two coordinating organic molecules [3]. This, which can be considered as a variable switch, can be actuated by tunneling electrons and show a quantum yield that vary in space and that can be related to the local density of states of the bonded and unbounded configuration.

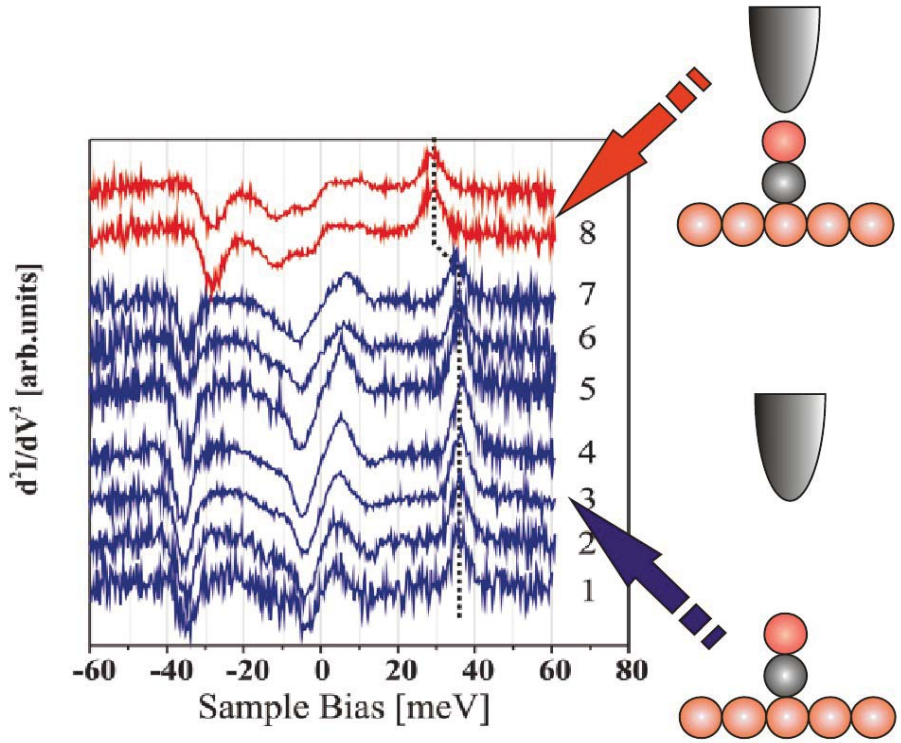

Figure 1. *Vibration spectra of individual CO molecules on Cu(111) at different tip-substrate distances ranging from tunneling to the point contact.*

References

[1] L. Vitali, S. D. Borisova, G. G. Rusina, E. V. Chulkov, K. Kern, Phys. Rev. B **81**, 153409 (2010)
[2] L.Vitali, R.Ohmann, K. Kern, A. Garcia-Lekue, T. Frederiksen, D. Sanchez-Portal, A. Arnau, Nano Letters **10**, 657 (2010)
[3] R. Ohmann, L. Vitali, K. Kern, Nano Letters DOI:10.102/nl1014348