Imaging and manipulation of molecular orbitals on metal surfaces with scanning tunneling microscopy

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Scanning tunneling microscopy (STM) allows to image molecular orbitals close to the Fermi energy by acquiring conductance maps. Furthermore, the STM can be employed to manipulate such molecular orbitals. Here, several mechanisms for such control for molecules adsorbed on a metal surface are presented. In the first, an additional Cu adatom is moved with the tip of the STM towards the molecule 4-[trans-2-(pyrid-4-yl-vinyl)] benzoic acid (PVBA) adsorbed on Cu(111). The local density of states is mapped before and after the manipulation indicating a change in the molecular orbitals upon attachment of the adatom to the molecule. In the second case, a self-assembled metal-organic complex composed of two PVBA molecules and a central Cu atom is excited by an electrical bias. This acts as an external stimulus causing the metal-ligand bond to alternate on a time-scale of milliseconds between a bonded and a non-bonded configuration. These two configurations reveal different molecular orbitals, which can be visualized by taking conductance maps. The quantum yield per tunneling electron to trigger a transition between the two states varies spatially and is related to the local density of states of the bonded and non-bonded configuration. Finally, the control of molecular orbitals by different binding geometries of molecules within a supramolecular structure will be presented.

References:

[1] Ohmann R., Vitali L., Kern K. Nano Letters, 10 (2010) 2995-3000.

Figures:

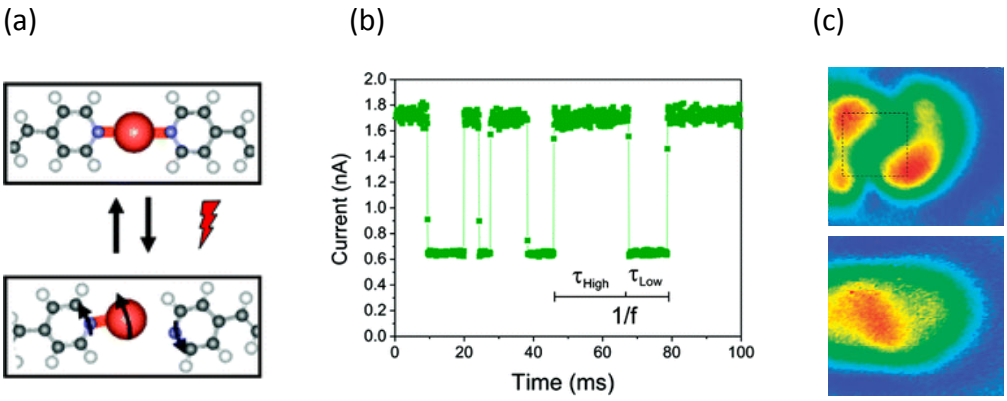

Figure 1: (a) Schematic of the electrically induced bond breaking and forming of a metal-ligand bond of $Cu(PVBA)_2$. (b) Current as a function of time indicating the alternation between the bonded and the non-bonded configuration. (c) Corresponding conductance maps of a bonded and non-bonded PVBA molecule (image sizes 18 x 20 Å²).