Dynamical bistability of a single PTCDA-STM junction:
A combined experimental and theoretical study

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A concept with fascinating potential applications is the creation of logic gates at the single molecule level. For this, however, a microscopic understanding of the adsorption behavior of the molecules on surfaces as well as their behavior under applied bias should be achieved. Furthermore, an additional factor to be clarified in order to facilitate the performance of logic operations in single molecules, are the physical mechanisms responsible for conformational or electronic changes in the molecule, which could thus change the output of a molecular-based device.
The scanning tunnelling microscope (STM) is a valuable and versatile tool for the study and manipulation of such nanoscale structures[1,2] and just recently the first single molecule logic gate was built with the help of an STM.[3] We will present a systematic study using STM on the cleaving and the switching of a perylene-3,4,9,10-tetracarboxylic-dianhydride (PTCDA) molecule on Ag(111). Using a minimal model Hamiltonian approach, the switching is shown to be related to a vibrational heating mechanism,[4,6] in which the tunneling electrons are inelastically scattered by vibrations, progressively exciting the relevant chemical bond. By combining this model with density-functional calculations, a good agreement with the experiments can be achieved.[4,5]
If the STM tip height is fixed, such a bistable molecule could be used as a simple memory element in which the high current state represents “1” while the low current state represents “0”. Alternatively, the tip height can be used as a second input resulting in a simple AND gate. Furthermore, since the energy needed to induce the switching is of the order of few hundred meV this logic gate could be stable at room temperature.

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