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Subject: Short scientific report - COST-STSM-CM0601-4580

STM manipulation of explosive compounds

The present mission which was carried out from July, 1st to July, 31st intended to investigate explosive compounds by means of the scanning tunnelling microscope (STM) in the laboratories of Prof. Roberto Otero, LASUAM, Universidad Autónoma de Madrid, Ciudad Universitaria de Cantoblanco, Madrid, Spain. One objective of this mission was also to establish a new collaboration of the home institute of the applicant Michaela Hager, Institute of Ion Physics and Applied Physics, University of Innsbruck, Austria, with the Spanish group.

A long desired aim is the controlled cleavage of chemical bonds by electrons, which is also the topic of the COST ECCL network. The studied molecule was pentaerythritol tetranitrate (PETN), which properties in the gas phase have been investigated in detail in Innsbruck from both experimental and theoretical side. To implement these results in the scientific aim of the ECCL network we carried out surface experiments by STM in Madrid. In brief, the explosive compound was heated in an external oven and then deposited onto highly orientated pyrolytic graphite (HOPG) and Cu(110). In figure 1 an image of HOPG after it was exposed to the target molecule is shown. It can be seen that the amount of PETN found on the surface is very small. On the contrary in figure 2 areas of self assembled PETN molecules on Cu(110) are visible.

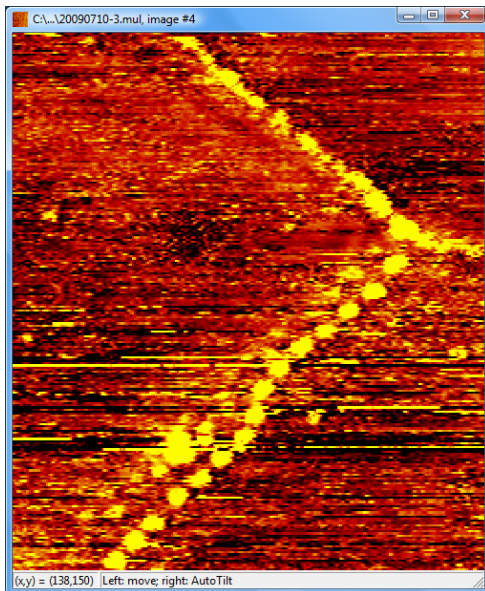


Figure 1: PETN molecules deposited onto HOPG, image size $500\text{\AA} \times 500\text{\AA}$

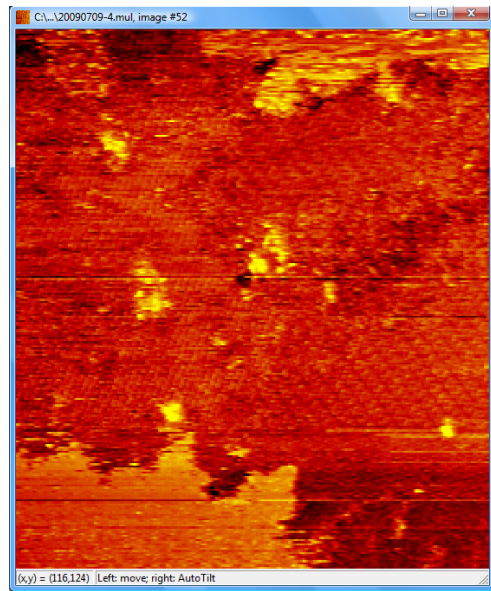


Figure 2: PETN molecules deposited onto Cu(110), image size $1000\text{\AA} \times 1000\text{\AA}$

Based on these first results we chose to concentrate on deposition of PETN onto Cu(110). We started a systematic investigation where we varied different experimental conditions, e.g. deposition temperature, and scanning temperature. We could demonstrate that for deposition and measurements at room temperature molecules tend to form rectangular islands with hexagonal arrangement that are transformed into a so-called striped phase only by measuring a second time over the same area. By deposition onto a cold sample and measuring at cold temperatures ($\sim -30\text{ }^\circ\text{C}$) it can be seen that the hexagonal phase is the first one to appear which then transforms into the striped phase under certain conditions. If the sample is too cold (below $-50\text{ }^\circ\text{C}$) the scanning current and voltage do not suffice to change the rectangular phase into the striped one. At around $-30\text{ }^\circ\text{C}$ it is still possible to change a rectangular island into a striped one by applying a voltage ramp to about 3 V. In figure 3 and 4 the two different phases can be seen.

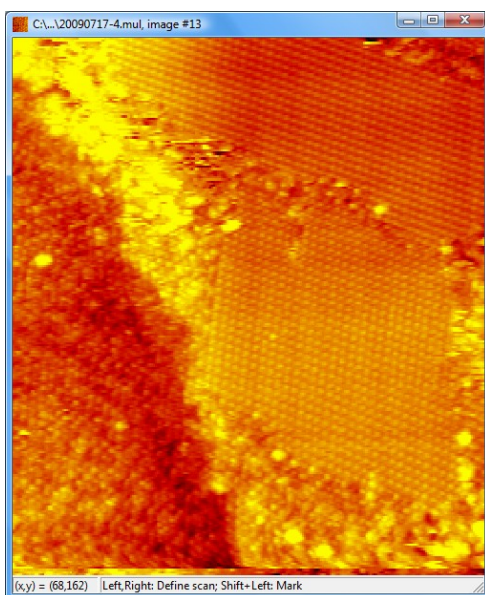


Figure 3: Rectangular ice lands image size $300\text{\AA} \times 300\text{\AA}$

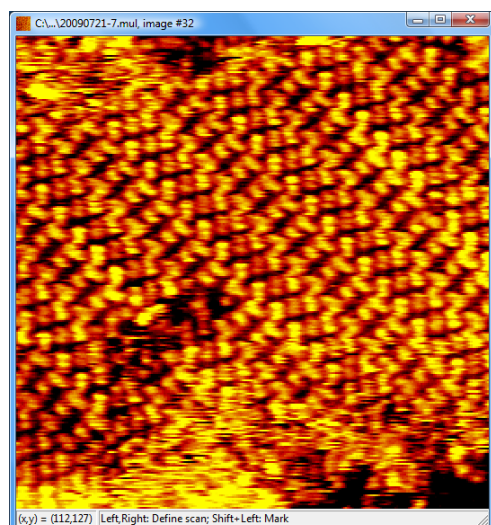


Figure 4: Striped phase image size $150\text{\AA} \times 150\text{\AA}$

The next step will be a detailed analysis of the large amount of data obtained during this successful STSM in the following weeks in collaboration with our colleagues in Spain. Due to the promising results we agreed to amplify the new collaboration between the two institutes.

A handwritten signature in blue ink that reads "Hager Michaela". The script is cursive and fluid, with the first letter of each word being capitalized and larger than the others.

Hager Michaela