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SCIENTIFIC REPORT

COST Action Number: CM0601
Host: Prof. Dr. Karina Morgenstern, Institut für Festkörperphysik, Abteilung Oberflächen, Leibniz Universität Hannover, Hannover (DE)
Period: from 22/09/2008 to 19/12/2008
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Purpose of Visit

Recently Scanning Tunneling Microscope - Inelastic Electron Tunneling Spectroscopy (STM-IETS) has been developed to measure the vibrational spectrum of a single molecule allowing STMs to be used as a tool for chemical analysis of single molecules. STM-IETS gives a new approach to chemistry on the single molecular level. The aim of this project was to focus on understanding electron induced isomerisation reactions of 4-anilino-4'-nitroazobenzene molecules on a metallic substrate. Prof. Morgenstern has a great experience in IETS. Her laboratory is well equipped and as such was perfect to elaborate this work.

Description of the work carried out during the visit

During the visit in Hannover, I focused on understanding electron induced isomerisation reactions of 4-anilino-4'-nitroazobenzene. The structure of the gas phase molecules obtained using geometry optimalization by means of energy minimalization AM1 algorithm is presented on Figure 1.

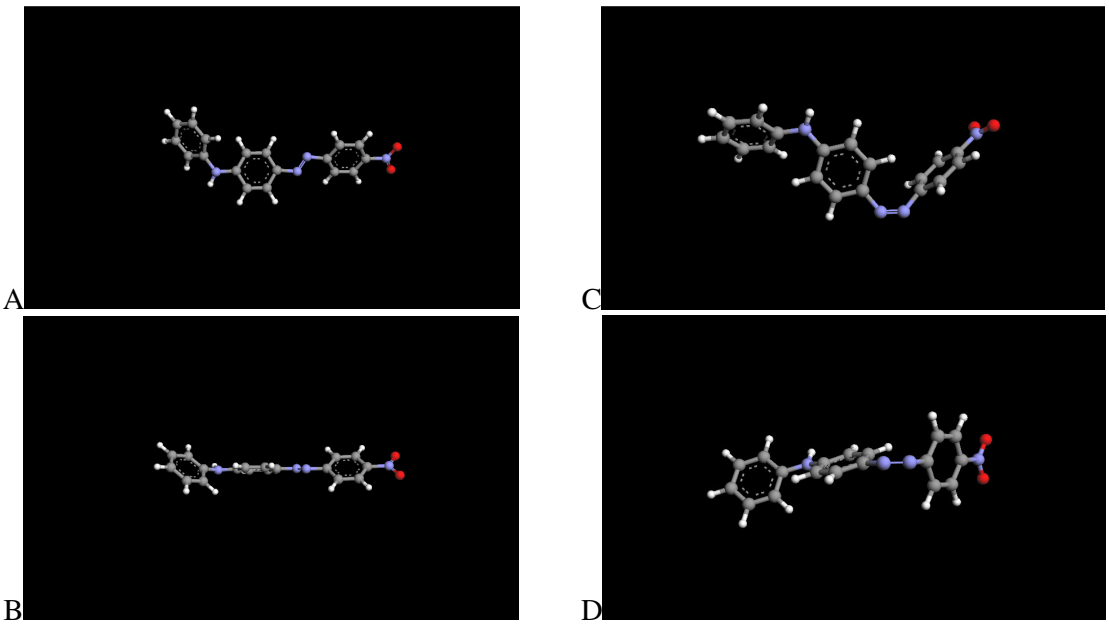


Fig. 1. Simulated structures of Cis (A, B) and Trans (C, D) isomers of 4-anilino-4'-nitroazobenzene. Images A and C show the view on the -C-N=N-C- plane, B and D show the view perpendicular to the mentioned plane.

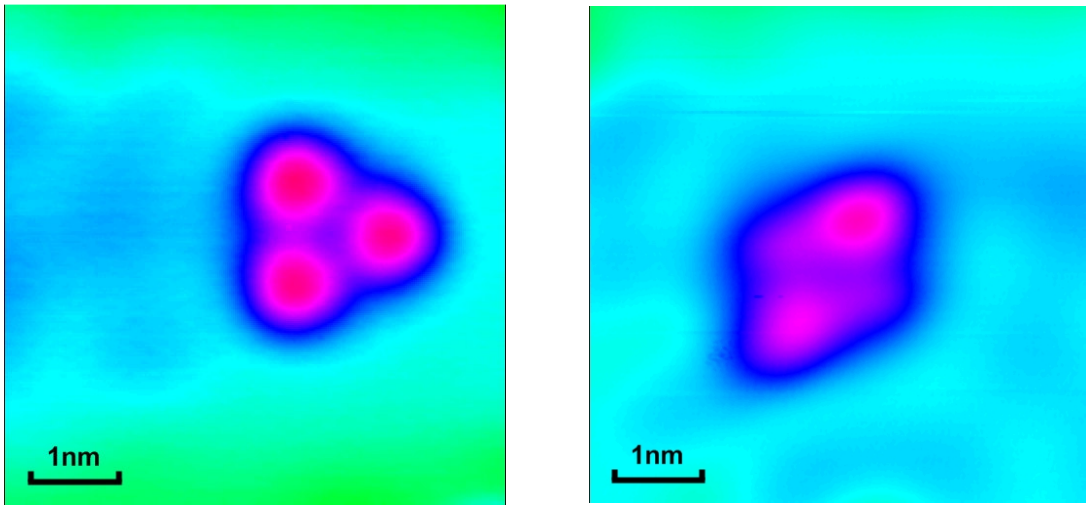
The experiment was performed with a low temperature STM. Low temperature is necessary to eliminate diffusion of the molecules due to thermal energy as well as to minimize the thermal broadening of the dI^2/dV^2 vs. V spectra.

It was essential that the substrates were perfectly clean and locally atomically flat. Such metallic surface was obtained by the standard sputtering/annealing procedure.

The molecules were sublimated in situ in UHV system onto the Cu(111) substrate. After this preparation, both Cis and Trans forms of the molecule were found on the surface. The isomerisation reaction was induced via electrons and light illumination.

Description of the main results obtained

The molecules were sublimated onto a substrate at a temperature of 100K from a Knudsen cell at the temperature of 400K and a pressure of 2.5×10^{-8}mbar. The base pressure in preparation chamber was at the level of 7×10^{-10}mbar. The obtained coverage was less than 0.05ML (as estimated from the STM images). Molecules at this temperature did not create



A B

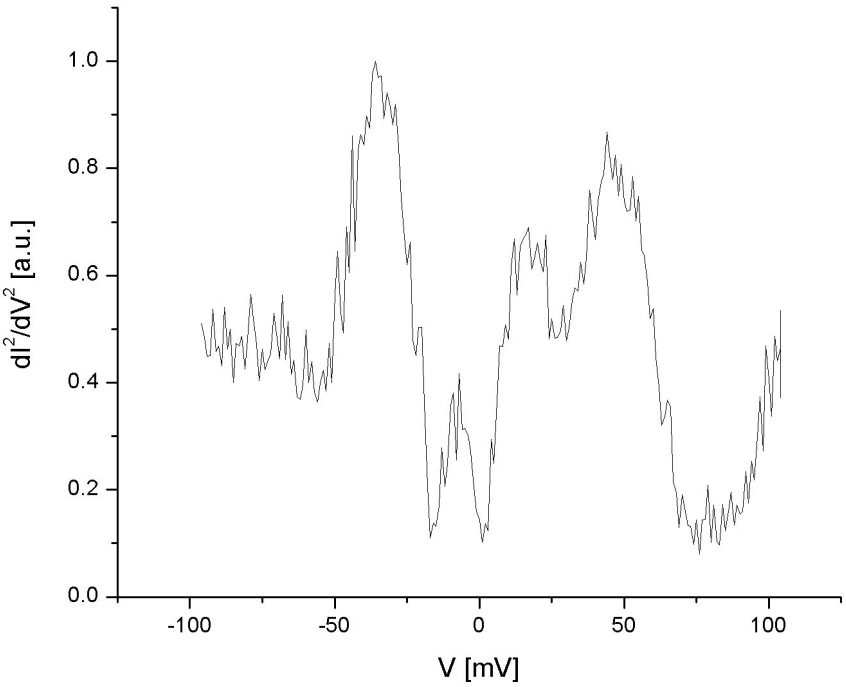
Fig. 2. STM image of Cis and Trans form of the 4-anilino-4'-nitroazobenzene.

any agglomerates. They were randomly placed on the surface. Two stable forms were identified on the sample (see Figure 2). The vibrational spectra were gathered over both species in order to help identifying the species structure which obviously differs from the structure in gas phase (see Figure 3).

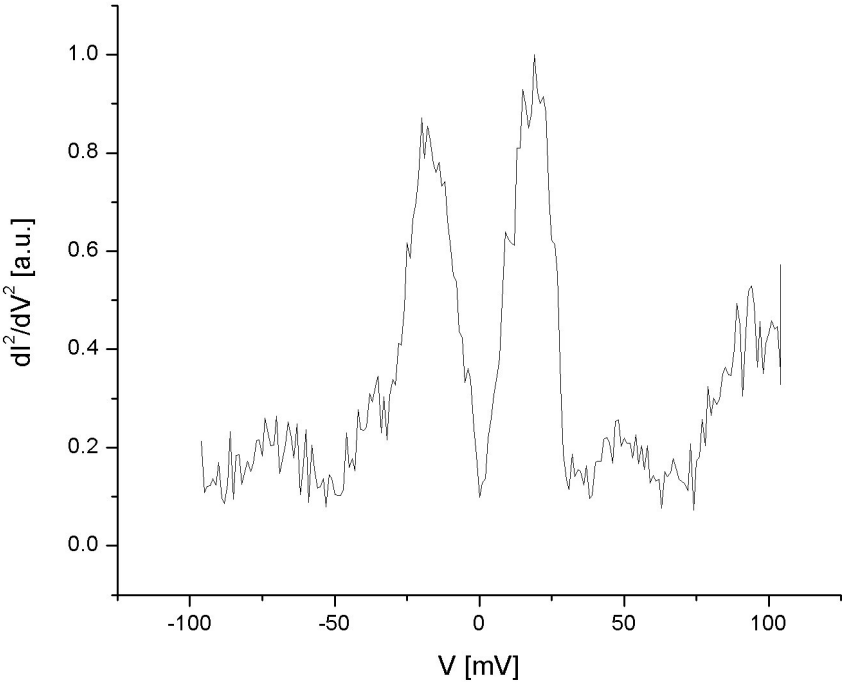
The electron induced isomerisation has been performed at different conditions in order to find the threshold. A threshold was found at approximately 200 mV, but the data are still being analyzed at present.

Isomerisation reactions were also induced by exposing the sample to unfiltered light from a mercury lamp. The heating effect as the reason of switching was excluded by an additional experiment with annealing the sample to the temperature reached during the illumination.

The wave lengths of light causing Cis to Trans and Trans to Cis transitions in gas phase are well known to be 332nm and 435nm respectively. The illumination with selected wavelengths in the range of 330-600nm, however, did not switch the molecules at all. This means that the energies necessary for the reaction are drastically different at the surface in comparison to the gas phase.



A



B

Fig. 3. dI^2/dV^2 vs. V spectra gathered over both species presented in figure 2 respectively.

Projected publications/articles resulting or to result from the STSM (if applicable)

The data obtained during my stay at the Leibniz University Hannover are analyzed at present time. It is planed to present them in the near future at scientific conferences. Moreover an article “Electron induced isomerisation of 4-anilino-4’-nitroazobenzene on Cu(111)” will be prepared for publication after completing the data with further calculations.