Abstract

In this thesis the substituted benzene molecules are studied on copper, gold and silver surfaces by means of low temperature scanning tunnelling microscopy (STM).

The adsorption geometry of phenyl rests, nitrobenzene and chloronitrobenzene molecules on Cu(111) is determined through the synergy between performed measurements and molecular dynamic calculations. The analysis shows that these molecules are adsorbed with the centre of phenyl ring being on the top of a copper atom. The qualitative comparison of STM images of phenyl rests and nitrobenzene molecules shows how the substitution of one hydrogen atom by one nitro group transforms the molecule from an insulator to a conductor.

The electron induced manipulation is utilised to change the adsorption geometry of nitrobenzene molecules on Cu(111) from the flat-lying to the up-standing bonding configurations on the surface. The measurements have pointed out, that the change of the adsorption geometry of nitrobenzene molecules is initiated by the ionisation of the molecule.

The cornerstone of this thesis is in the investigation of the isomerisation inside single chloronitrobenzene and dichlorobenzene molecules on different surfaces. While the former are studied on Cu(111) and Au(111), the latter are examined on Ag(111). As a result of the induced chemical reaction, the positions of chlorine and one hydrogen atom are exchanged. The isomerisation is completely described by the determination of the corresponding reaction mechanism. This chemical reaction is initiated by appropriate molecular vibrations, which are necessary for forcing chlorine and hydrogen first to come near and then to mutually exchange their positions.

The performed experiments have shown that the excitation of the isomerisation occurs only in the case where two vibrations inside the single molecule are initiated at the same time. One of these vibrations is always the C-Cl one. No significant differences are found in the excitation mechanism for the different surfaces investigated.

The control experiments, performed on chloronitrobenzene molecules on Cu(111) and Au(111), have shown that the chlorine atoms in isomerised molecules are chemically bound.

It is also possible to remove and chemically bound chlorine atom from a chloronitrobenzene to a nitrobenzene molecule.

Finally, the rotation of chloronitrobenzene molecules on Au(111) has been investigated. It has been found that the underlying reaction mechanism is based on the excitation of a molecular vibration.