# Adlayer Structures of Fullerene Derivatives on Au(111)

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Fullerenes have been studied extensively because of their unique physical and chemical properties. Understanding the adlayer structure of fullerene derivatives on metal surfaces is important in various fields of surface science. In the present work, we investigated the adlayer structures of fullerene derivatives on Au(111) in solution and in vacuum.

Figures 1a and 1b show the chemical structures of $C_{60}$-$C_{60}$ dimer ($C_{120}$) and $C_{60}$ malonic acid, the adlayer structures of which were investigated. The adlayers of $C_{120}$ and $C_{60}$ malonic acid were prepared by immersing the Au(111) surface into saturated $C_{120}$ benzene solution and $C_{60}$ malonic acid benzene solution respectively. EC-STM measurements were carried out in 0.1 M $HClO_4$ solution. STM and LEED measurements were performed in vacuum. All potentials are reported with respect to a RHE.

***$C_{120}$*** Figure 2 shows an EC-STM image of a $C_{120}$ adlayer observed at 0.75 V on Au(111) in 0.1 M $HClO_4$ . Ordered molecular arrays were observed on the terrace. Each $C_{120}$ molecule is seen as a set of two bright spots separated by a distance of *ca.* 0.96 nm, which is in good agreement with the X-ray crystal structure of the $C_{120}$. Adlayers of $C_{120}$ molecules on the Au(111) surface were found to form $(2\sqrt{3} \times 4\sqrt{3})R30°$ and $(2\sqrt{3} \times 5\sqrt{3})R30°$ structures.[1] The same symmetries and the same molecular arrangements were observed on the adlayer in vacuum by LEED and STM, indicating that water exert little influence on the formation of the $C_{120}$ adlayer on Au(111). It is noteworthy that the electronic structure of $C_{120}$ molecules adsorbed on Au(111) can be observed in vacuum by STM.[2]

***$C_{60}$ malonic acid*** Figure 3 shows a high resolution EC-STM image of a $C_{60}$ malonic acid adlayer observed at 0.23 V on Au(111) in 0.1 M $HClO_4$. The STM measurment revealed that the $C_{60}$ malonic acid adlayer on Au(111) formed an ordered structure. The rhombus drawn by solid lines is the unit cell of the ordered structure. The length of each side of the rhombic unit cell is *ca.* 1.0 nm and the sides cross each other at an angle of either 60° and 120°. All side of the unit cell are tilted by *ca.* 5° with respect to the direction of the Au rows. The unit cell indicated that the $C_{60}$ malonic acid adlayer formed an incommensurate structure. In the STM image, a set of two small spots, shown by white circles, was observed between adjacent big spots along the direction of the arrow A. Taking into account the commensurate structure of $C_{60}$ adlayer on Au(111), -COOH groups of $C_{60}$ malonic acid played an important role in the formation of the adlayer. Detailed analysis of the STM image revealed that each big spot and each set of two small spots might be C60 cage and -COOH groups of $C_{60}$ malonic acid, or $C_{60}$ malonic acid and water. LEED and STM measurements indicated that $C_{60}$ malonic acid adlayer in vacuum formed an incommensurate adsorbed structure, and the symmetry and the molecular arrangements were different from those in solution.

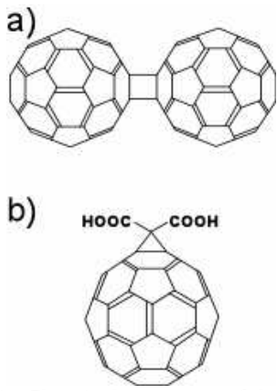


Figure 1 Chemical structures of the $C_{60}$-$C_{60}$ dimer ($C_{120}$) (a) and the $C_{60}$ malonic acid (b).

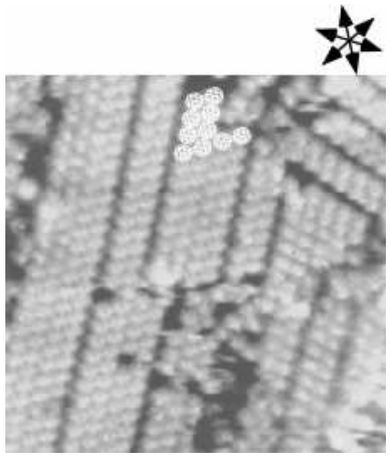

Figure 2 STM image of a $C_{120}$ adlayer on a Au(111) surface in 0.1 M $HClO_4$ acquired at 0.75 V versus RHE. ($23 \times 23$ nm$^2$)

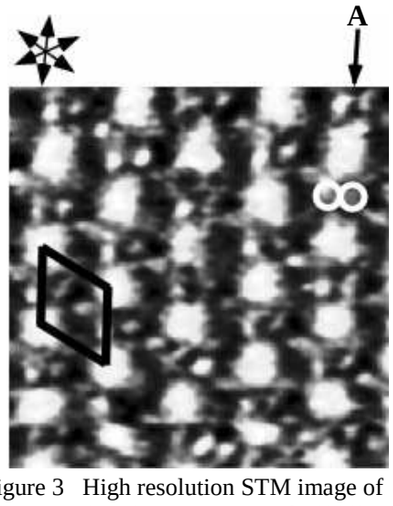


Figure 3 High resolution STM image of a $C_{60}$ malonic acid adlayer on a Au(111) surface in 0.1 M $HClO_4$ acquired at 0.23 V versus RHE. ($4.9 \times 4.9$ nm$^2$)

REFERENCES

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