STM study on the interactions of individual $C_{60}F_{18}$ molecules with the Si(111)-7×7 surface

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The use of organic nanoscale self-assembled structures compatible with Si-based semiconductor system offers the perspective of tuning their electronic functionality by redesigning the molecular components. Therefore, carbon fullerenes and their derivatives are promising in fabrication of electro-active elements in solar cells and active layers in organic thin film transistors. Among others, highly fluorinated fullerene is worthy from the above-mentioned viewpoint. We have used scanning tunneling microscopy (STM) and ***ab initio*** pseudopotential calculations based on density functional theory (DFT) to study initial stages of individual $C_{60}F_{18}$ molecules adsorption on a Si(111)-7×7 surface. In contrast to $C_{60}F_{46\div48}$ molecules (which have been studied before [1]) tortoise-shaped polar (>9.0 Debye) $C_{60}F_{18}$ molecules are very asymmetrical: all the 18 fluorines are bound to one hemisphere of C_{60} only and flatten its shape.

All experiments were carried out at room temperature using a ultra high vacuum STM (base pressure 2×10^{-11} Torr) equipped with standard surface preparation facilities. The deposition of $C_{60}F_{18}$ molecules has been performed from Knudsen cell on a Si(111)-7×7 surface kept at room temperature.

It is found that polar fluorinated carbon fullerene has large binding energy on a corner hole site of Si(111)-7×7 surface due to induced polarization on the Si surface. Calculations also suggest that $C_{60}F_{18}$ molecule binds on the Si surface with F atoms interacting with the surface and that no image should be seen in STM at the bias used from regions of the molecule as well as Si surface where F atoms exist. The high binding energy of F atoms on adatom and rest sites of Si surface and the appearance of black spots in images, lead us to conclude that during the time of the experiment, F atoms tend to migrate to the surface. Such a possibility has been known in studies of other higher fluorinated fullerenes [1], but in C60F18, this tendency is weaker due to the higher stability of C60F18.

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