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Deuteration of C_{60} on a highly oriented pyrolytic graphite surface

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Abstract. Reactions on carbonaceous surfaces play an important role in processes such as H_2 formation in the interstellar medium. We have investigated the adsorption of C_{60} molecules on a highly oriented pyrolytic graphite (HOPG) surface and then exposed them to a beam of deuterium atoms in order to investigate the formation of deuterated fullerenes. Scanning tunneling microscopy (STM) was used to probe the adsorbed molecules and their deuteration. Deuteration of C_{60} films results in increased thermal stability of the film, relative to films of pristine C_{60}, along with an evolution towards higher deuterated species. The STM data provide confirmatory evidence for the formation of deuterated fullerene species.

Keywords. physical data and processes: astrochemistry - methods: laboratory - ISM: molecules

Overview

Buckminsterfullerene, C_{60}, is present in the interstellar medium (ISM) in regions near hot stars (Sellgren *et al.* 2010). It has also been identified (Campbell *et al.* 2015) in its ionized form as a carrier of diffuse interstellar bands (DIBs). Authors (Berné & Tielens 2012) are proposing a top-down approach to form C_{60} from polycyclic aromatic hydrocarbons (PAHs) in interstellar environments. Experimental (Thrower *et al.* 2012) data suggest that the latter can act as catalysts for H_2 formation. It is therefore also of interest to study C_{60} hydrogenation on carbonaceous grains as a substrate for catalytic reactions in the ISM, in particular in photo dissociation regions (PDRs). The H_2 abundances in the ISM are determined by the equilibrium between formation (*e.g.* hydrogenation) and destruction (*e.g.* exposure to UV radiation). For C_{60} films, deuteration is found to lead to enhanced thermal stability (Löffler *et al.* 2007). C_{60} is also known to be stable against UV-induced fragmentation. These two factors may lead to an evolution of carbonaceous grains to produce larger dust structures over time. We have employed an HOPG surface as a carbonaceous interstellar grain analogue. Deuteration of the C_{60} film was performed to simulate hydrogenation that occurs in H-rich environments.

An HOPG sample was cleaved under atmospheric conditions and directly transfered to an ultra high vacuum (UHV) chamber with a base pressure of ca. 5×10^{-10} mbar. The sample was heated to 1200 K to desorb any contaminants. For the deposition of C_{60}, C_{60} powder (Sigma-Aldrich, >99%) was placed inside a crucible of the Knudsen cell and thermally evaporated at 633 K. The HOPG sample was held at *ca.* 340 K during deposition. C_{60} films were exposed to a D-atom beam produced by a hot capillary thermal cracking source as described in Tschersich (2000) (MBE komponenten; HABS). During

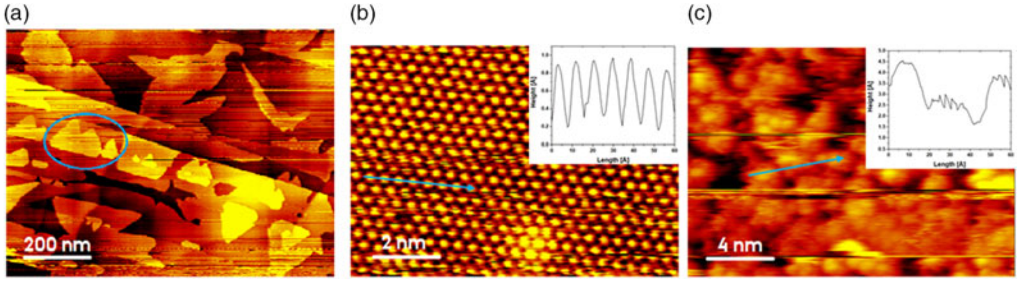

Figure 1. STM images of (a) pristine C_{60} on HOPG forming a film with islands (example of an island is marked with the blue oval shape) (I_t=2.270 nA, V_t=2668.1 mV), (b) picture of pristine close-packed C_{60} on HOPG with molecular resolution (I_t=1.230 nA, V_t=1903.7 mV) and (c) C_{60} films after exposure to a fluence of 3×10^{17} D atoms/cm^2 with molecular resolution (I_t=0.350 nA, V_t=1535.6 mV). In the inset of (b) and (c) are presented the line scan profiles in the positions corresponding to the blue arrows.

D-atom exposure the HOPG temperature was < 340 K. An Århus-type STM was utilized to characterize the surface and adsorbed molecules.

In Fig. 1(a) C_{60} islands on an HOPG surface exposed to approximately 5 monolayers (ML) of C_{60} are displayed - the blue oval outlines an example island. The smaller scale image in Fig. 1(b) reveals that C_{60} molecules are arranged in a close-packed hexagonal structure with a height of *ca.* 1 Å (inset Fig. 1(b)). Following exposure to a D-atom beam fluence of 3×10^{17} atoms/cm^2, the well ordered structure displayed in Fig. 1(b) is replaced by more disordered and inhomogeneous structures as the one displayed in Fig. 1(c). The height of these structures is locally larger than 4 Å as can be observed in the inset of Fig. 1(c). The bright protrusions in the image are ascribed to D-atom functionalization of individual C_{60} molecules, as well as to D-atom induced intermolecular sticking and clustering. This corresponds well with the observation of higher mass species and increased desorption temperature for hydrogen functionalized C_{60} films, as revealed through temperature programmed desorption measurements (see Thrower *et al.* in this volume).

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