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Investigation of the hydrogenation of pentacene

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Carbonaceous surfaces are known to act as catalysts for the formation of molecular hydrogen in the interstellar medium [1,2]. Molecular hydrogen is the most abundant molecule in the universe and it controls the chemistry of the interstellar medium. Hence, the formation of molecular hydrogen is the first step in the evolution of the chemical complexity of the interstellar medium.

Observations correlate the abundance of polycyclic aromatic hydrocarbons (PAHs) to an increased rate of H_2 formation [3]. PAHs and HPAHs are closely linked to the carbonaceous grain population although PAH interaction with grains is still poorly understood. Experiments and theoretical calculations indicate that PAHs play a role as catalysts for H_2 formation [4] and addition of hydrogen to PAHs pushes the molecule away from a planar geometry [5]. Here,we investigate reactions between pentacene and atomic hydrogen. Our goal is to examine the carbon sites at which incoming H atoms are most likely to bind, and to study how the morphology and reactivity of the pentacene molecule changes as the degree of superhydrogenation increases.

A monolayer of pentacene was prepared under ultra-high vacuum conditions on a Au (111) surface and then exposed to a controlled fluence of hydrogen atoms. X-ray photoelectron spectroscopy was used to characterize the system by tracking chemical shifts in in the C1s and Au4f core levels.

After hydrogenation, a chemical shift was observed for the carbon core level electrons. This indicates that the sp^2 carbon sites change to a sp^3 hybridisation after hydrogen exposure. Furthermore, there is evidence for more than one type of sp^3 hybridised carbon site. Chemical shifts in the gold core levels were observed firstly after dosing of pentacene and again after hydrogen exposure. The latter could indicate Au-C bond formation simultaneous with new C-H formation on the pentacene molecule or a Au-H interaction, or both. Combining this data with STM images and DFT calculations will help us understand the dynamics of hydrogen addition to the pentacene molecule and elucidate a route towards superhydrogenation of the PAHs in the interstellar medium.

References

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