Electronic structure and dynamics of adsorbed and condensed phase PAHs

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Description:
Polycyclic aromatic hydrocarbons (PAH), a wide class of organic molecules consisting of multiply fused aromatic rings, are of great importance in many research fields such as combustion and environmental chemistry, material science and astrochemistry. PAHs have been proposed as (terrestrial and extra-terrestrial) precursors to extended carbon networks including carbon nano-tubes and fullerenes. Self-assembled monolayers of PAHs based on organic semiconductors are particularly promising for the fabrication of organic field effect transistors, sensors and optoelectronic devices.

In the astrochemical context, PAHs are ubiquitous in the interstellar medium (ISM) and are expected to exist in the condensed phase as precursors to small graphitic grains, adsorbed onto carbonaceous grains or acting as condensation nuclei for icy grain mantles, playing a crucial role in heterogeneous chemistry. As such, the relatively unexplored dynamic behaviour of low-coverage adsorbed PAHs on carbon-based substrates is of great interest both in material science applications and in elucidating astrophysical processes on carbonaceous grains with evidence of the continuous diffusion of benzene (the simplest aromatic building block of PAHs) on graphite [1,2]. On the other hand morphological effects at high coverages of amorphous phases of PAHs are also of considerable interest with evidence of the electronic states of benzene being strongly perturbed by intermolecular interactions [3] and there are concentration dependent effects within an ice matrix [4], which will be significant in describing photochemical processes involving PAHs.

This project will consist of a two-fold complementary study involving:

1) A systematic surface dynamics investigation of PAHs of different sizes and symmetries via acquisition and analysis of data from neutron scattering measurements and DFT calculations to investigate the structure and energy landscape of PAHs adsorbed on graphite surfaces. The approach is applicable to material science and bare-grain astrochemical processes, as graphite forms an ideal carbonaceous grain surface analogue.

2) Spectroscopic investigations of the electronic states of amorphous and crystalline phases of thin films of the same PAHs used in (1) with different sizes and symmetries and their interaction with polar and non-polar molecules, applicable to grain-ice mantle interactions in the ISM. This work will involve vacuum ultraviolet spectroscopy measurements at the ASTRID2 synchrotron Facility, Denmark.

We seek an enthusiastic and highly motivated candidate with a willingness to learn and develop ultra-high vacuum laboratory techniques to acquire high quality systematic laboratory data and perform computational data analysis.

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References:


Qualifications required:

A First Class or Upper Second class MSci degree in Physics, Chemistry or related discipline. Previous experience in vacuum technology and surface science is desirable.