The Structure of Metal-Organic Interfaces

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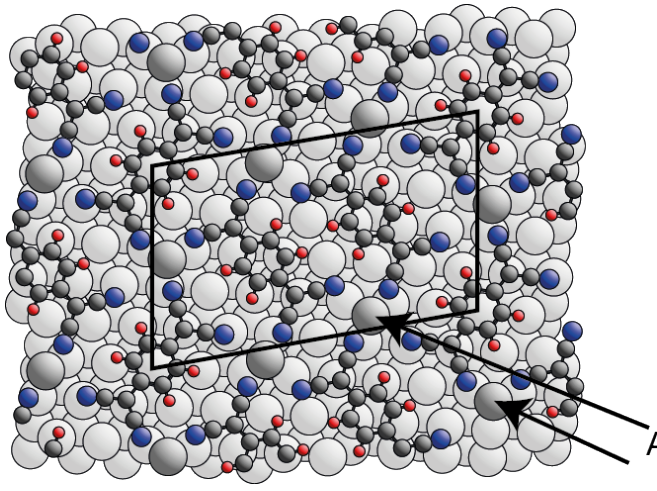
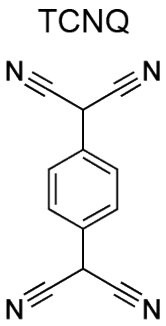
Metal/organic interfaces (MOIs) play a crucial role in a range of practical applications. They strongly influence the performance of organic electronic devices (OEDs), but they also play an important role in a range of corrosion inhibitors and in the biocompatibility of medical implants. The functionality of these interfaces is determined by the electronic and chemical properties of these interfaces, but following the axiom that structure determines function, we must first understand the structure of these interfaces. The objective of this project is to determine some of these structures, using two novel techniques exploiting synchrotron radiation and, in particular, the world-wide unique beamlines for these measurements at the UK's national synchrotron radiation facility, the Diamond Light Source, located south of Oxford on the Harwell Innovation Campus. Specifically, normal-incidence X-ray standing waves (NIXSW), a method first developed by the Warwick group, allows us to determine the conformation and adsorption height of adsorbed molecule. Experiments so far have also provided indirect evidence that in many cases the interaction of the molecule with a metal surface extracts metal atoms to create two-dimentional metal-organic frameworks on the surface (see the figure), rather than simply a molecular overlayer. NIXSW is 'blind' to the presence of these adatoms, but Surface X-ray diffraction (SXRD) is sensitive to the presence of the 'heavy' metal adatoms within the molecular layer, providing direct evidence of their presence and location. We have performed proof-of-principle experiments to demonstrate the efficacy of this combined approach and this project will extend and apply this combination of methods to fully establish the new methodology.

This is a collaborative project part-funded by Diamond Light Source, providing the student with the considerable advantage of the experience of working at this state-of-the-art national facility as well as within the University of Warwick. The joint funding leads to an enhanced value of the student stipend (£17,246 in Year 1) and additional funding for Warwick-Diamond travel and subsistence and conference attendance.





Example of a 2D-metal organic framework formed by the adsorption of the TCNQ ((7,7,8,8-tetracyanoquinodimethane) on a Ag(111) surface determined in this work.

TCNQ is a prototypical electron acceptor molecule used in organic electronics.