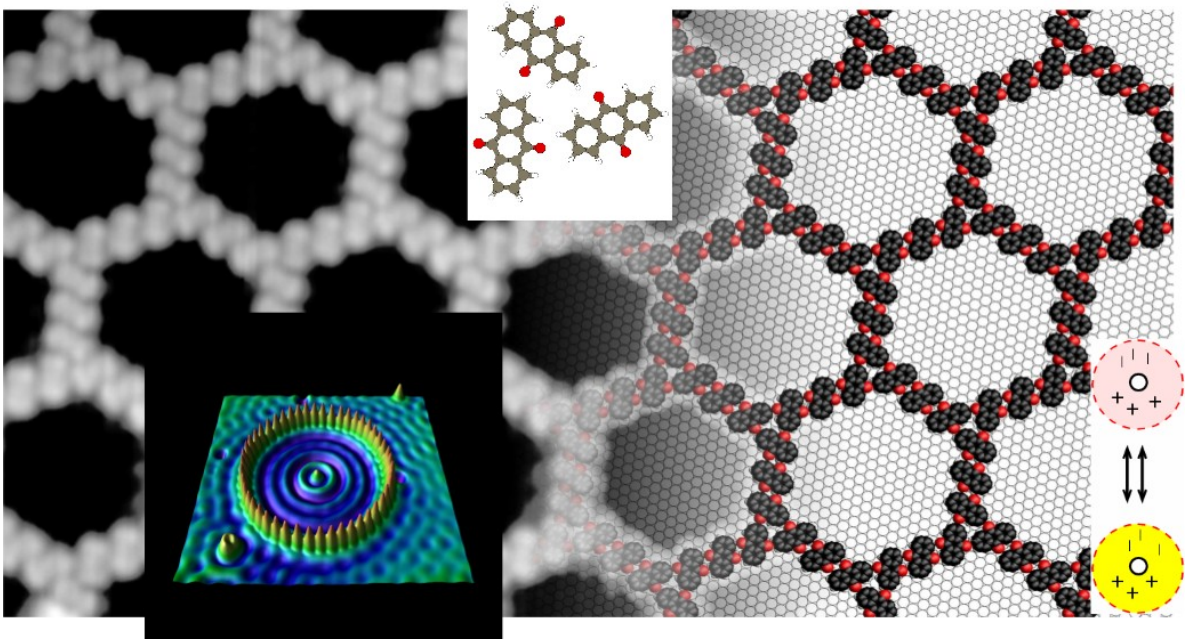
Understanding molecular assembly at surfaces: a modern density-functional-theory exploration



Background
An important goal of surface science is to control the properties and function of organic-molecular structures that are adsorbed on surfaces. For example, in green technology, we seek to engineer highly porous networks that can trap pollutants at the huge internal surfaces which themselves must be almost inert. To grow such systems it can be advantageous to first form dilute overlayers that may nucleate a favorable assembly of the porous structure.

In practice, the goal of molecular-system control means understanding the nature and balance of interactions and seeking insight on how this balance depends, for example, on the molecular geometry, mutual organization, and surface properties. Surface and molecule understanding is also important in nanoelectronics, to affect a switching between different molecular states, and in photovoltaics, to improve the charge transfer rate to a substrate.

The figure shows an example, anthraquinone molecules on a Cu(111) surface, of an overlayer assembly where sparseness emerges from a subtle balance of forces. The weak chemisorption of the molecules is enhanced by - but not always dominated by - the van der Waals attraction (illustrated in the rightmost insert). It provides experimentalists with an opportunity for a direct observation of the molecular assembly (left part of figure). Such measurements are highly valuable for a modern density functional theory characterization (right part of figure). We can, for example, compare results for the line segments, vertex groups (top insert), and the substrate-electron interference effects (leftmost insert) that set the pore sizes in this self-assembly case. From such validation, we can gain trust in modern density functional theory description and can proceed to benefit from the enormous insight that this theory provides. For example, by correlating structural motifs with the spatial variation in binding contributions we can simplify engineering of a better molecular function.

Goals
The aim of the project is to compute and understand the competition between van der Waals and other electron-interaction effects for molecules at surfaces. We focus on problems where we have access to detailed measurements through international collaborations.

Master-thesis work
You will learn to understand and use modern, so-called nonlocal, density functional theory which is emerging as a new general-purpose tool for materials-theory exploration. You will be running calculations on Chalmers as well as national computer clusters and you will have world-unique access to tools for mapping the spatial signatures of the adsorption and of intermolecular attraction. From the mapping you can help start an exploration of improved control of molecular interaction and switching processes.

Master-thesis target group
The master-thesis projects is suited for students in the Chalmers nano, materials, or physics programs. It is also open for GU physics students.

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