SPECIAL SEMINAR
Wednesday 20/03/2018 11:00 am
Building 211, seminar room

SPEAKER:

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TOPIC:

An adventure with a phenyl ring: controlling energy alignment at semiconductor interfaces

The alignment of energy levels between two adjacent phases is a critical consideration for numerous fields, from catalysis, via electrochemistry and up to electronics. Especially, for electronics, interface properties are as important as, and often more than, the bulk properties (such as mobility and energy gap). At interfaces, a chemical gradient translates into an electro-potential profile, forming potential barriers and wells,\(^1\) which are the functional-core of diodes, transistors, and almost any (opto) electronic device. Molecular monolayers are now commonly used to tailor interfacial electric fields toward optimizing the performance of organic electronic devices such as solar cell, sensors and flexible electronics. But can we translate this empirical success into a set of design rules to tailor the interfacial potential step at our wish?
Molecular adsorption onto H-terminated Si (oxide free) provides an excellent testbed to identify the chemical ingredients of surface/interface polarization because of its rich surface chemistry and high-quality monolayers adsorbed on it.\(^1\) I will specifically focus on \(\sim 1\) nm long, styrene-like molecules, forming Si-monolayer / metal junctions, with mercury or lead as a top metal. This family of molecules include the three basic design elements for controlled electrostatics: a polarizable element (phenyl ring) an insulating buffer (alkyl segment) and various substituents (‘hetero-atoms’). I will demonstrate how the role of the hetero-atom varies depending on its position in the molecule: it can serve as i) charge source / sink,\(^2\) ii) shift the frontier orbitals\(^4\) and / or iii) dictate the degree of hybridization between molecule and substrate energy levels.\(^3\) Another tricky aspect is the ‘chemical softness’ of the molecules. If the soft element (phenyl ring, lone-pair atom) is located in an internal position it will help developing a large dipole,\(^2\) however, at terminal positions, it will facilitate charge-rearrangement with the adjacent solid-phase,\(^3\) an effect that often reduces the net dipole.\(^4\) This study provides a systematic tool-box for controlling energy alignment at molecular / solid interfaces.\(^1\)