



SEMINAIRE ISMO

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Self-Assembly of Organic 2D Materials on Transition Metal Surfaces

Extended materials consist of organic molecules fall between 'hard' and 'soft' materials categories, and presenting bare promising novel and useful functionalities. Their growth through self-assembly is, however, not well understood due to the lacking of a detailed understanding of an accurate account of different operative forces, which are responsible for the assembly of materials with varying physical/chemical properties.

I will present results of a detailed computational study of the adsorption of selected groups of organic molecules on metal surfaces with varying geometries and elemental composition. The targeted systems have the potential to serve as efficient devices for solar energy harvesting and for solid-state lighting (light emitters).

The computational studies use both standard density functional theory (DFT) as well as exploiting the inclusion of dispersive forces (Van der Waals interactions), with the aim of obtaining the effects of dispersive forces and their dependence on the surface chemical properties. I will present the results on how the interface characteristics between the organic materials and metal surfaces change with the characteristics of molecules, the degree of reactivity, as well as the geometry of the surface. The results obtained for the adsorption of the acenes, the thiols and those molecules with CN groups on seven transition metal surfaces (Au, Ag, Cu, Ni, Pd, Pt and Rh) will be presented.

**Attention !
Jour inhabituel**

Vendredi 11 juillet 2014 à 11h
Bât 210 – Amphi 1 (2^{ème} étage)
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