Organic materials/metal surfaces Interface Characteristics: Role of van der Waals interactions

Abdelkader Kara
Department of Physics, University of Central Florida

Extended materials consisting of organic molecules fall between 'hard' and 'soft' materials categories with 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.

The computational studies use both standard density functional theory (DFT) as well as exploiting the self-consistent 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 surfaces. The results obtained for the adsorption of acenes, thiols and those molecules with CN groups on several transition metal surfaces (Au, Ag, Cu, Ni, Pd, Pt and Rh) will be presented.