

Abnormal Work Function Modification at the Interface between Organic Molecule and Solid Surfaces

**Ji-Hoon Kim¹, Jae-won Seo¹, Hyeeseung Kang¹, Jeong-Kyu Kim¹,
Jeong Won Kim², Hangil Lee³, Young-Kyung Kwon¹, and Yongsup Park¹**

¹Department of Physics and Research Institute for Basic Sciences, Kyung Hee University, Seoul 130-701,
²Korea Research Institute of Standards and Science, P.O. Box 102 Yuseong, Daejeon 305-600 Department of
Chemistry, ³Sookmyung Woman's University, Seoul

Using both experimental and theoretical approaches, we have investigated the adsorption properties of an organic molecule (HATCN), which is used in OLEDs as an efficient hole injection layer, on metal and inert surfaces. We have also studied the structural and electronic properties of such interfaces and the dependences on deposition thickness. We have observed different trends in work function changes with different surfaces. Our photoelectron spectroscopic measurements have revealed an abnormal phenomenon in HATCN on a metal (Cu) surface: the work function decreases at lower coverage (~monolayer) of HATCN on a metal (Cu) surface, but it increases back and becomes higher than that of a bare Cu surface at higher coverage. It has, on the contrary, been observed that the work function of graphene surface just increases as the HATCN coverage increases. Our first-principles density functional calculations has not only verified our experimental observations, but also disclosed the underlying mechanism of such abnormal and different work function behaviors. We have found that the change in work function results from mutual polarization induced by the geometrical deformation and the bond dipole formed at the interface due to the charge redistribution. At low coverage of HAT-CN on Cu substrate, the former reduces the work function significantly by pulling down the vacuum level, while the latter tends to push up the vacuum level resulting in the work function increase.