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Electron spectroscopy study of interface electronic structures of 1,4,5,8,9,11hexaazatriphenylene-hexacarbonitrile on Cu(111) surface

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Recently, 1,4,5,8,9,11-hexaazatriphenylene-hexacarbonitrile (HAT-CN) has been highlighted as an effective buffer layer in organic light emitting diodes (OLEDs). We investigated the interface electronic structure of HAT-CN on Cu(111) single crystal surface using in-situ x-ray, uv photoemission spectroscopy (XPS and UPS respectively) and near edge x-ray absorption fine structure (NEXAFS). The work function of Cu(111) was reduction from 4.91 eV to 4.03 eV was observed when about 0.2-nm thick HAT-CN was deposited by thermal evaporated. However, when more HAT-CN was deposited the work function started to increase up to 5.33 eV at the molecular film thickness of 9.0 nm. The highest occupied molecular orbital (HOMO) was found at 3.77 eV below the Fermi level at this thickness. We will discuss these changes in WF in the context of metal-molecule charge transfer and resultant interface dipole formation as well as the reorientation of the molecule with increasing thickness.