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Mechanism of workfunction modification on HAT-CN/Cu(111) interface: *ab initio* study

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Using *ab initio* density functional theory, we study the structural and electronic properties of interface between Cu surface and highly electron withdrawing hexaazatriphenylene-hexanitrile (HAT-CN) known as an efficient hole injection layer for organic light emitting diodes (OLEDs). We calculate the equilibrium geometries of the interface with different HAT-CN coverages. Usually, some of C-N bonds located at the edge of the HAT-CN molecule are deformed toward Cu atoms resulting in the reconstruction of Cu surface. By analyzing the electron charge and the potential distributions over the interface, we observe the formation of surface dipoles, which modify the work function at the interface. Such dipole formation is attributed to two origins, one of which is a geometrical nature and the other is a bond dipole. The former is related to structural deformation mentioned above, whereas the latter is due to charge transfer between organic and metal surface.