Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Structural and Electronic Properties of Interface between Metal and HAT-CN Molecule[1] YOUNG-KYUN KWON, JI HOON KIM, YONGSUP PARK, Kyung Hee University — Using *ab initio* density functional theory, we study the equilibrium structures and electronic properties of interface between metal surface and organic molecule, called 1,4,5,8,9,11- hexaazatriphenylene-hexacarbonitrile (HAT-CN), which is known for a strong electron acceptor and used as an efficient hole injection layer for organic light emitting diodes. We consider Ca (111) and Cu (111) surfaces, on which HAT-CN is placed. The geometrical and electronic properties of the interfaces are significantly different when HAT-CN is on one metal surface than when it is on the other. We find that the nitrogen atoms at the edge of HAT-CN have stronger interaction on metal surfaces than other atoms in the molecule. Due to the resultant charge transfer between the HAT-CN molecule and the metal surface, the surface dipole is formed at the interface. We discuss the dependence of the work function on the surface dipole formation and compare with the experimental results.

[1]This work was supported partly by NRF of Korea grant KRF-2009-0074951

Young-Kyun Kwon
Kyung Hee University

Date submitted: 20 Nov 2009 Electronic form version 1.4