SF3-002

Ab initio Study of the Structural and Electronic Properties of HAT-CN/metal interfaces for OLED Applications

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Using *ab initio* density-functional theory, we have investigated the geometrical and electronic structures of interfaces between a metal surface (Ca, or Cu) and a highly electron withdrawing hexaazatriphenylene-hexanitrile (HAT-CN) molecule known as an efficient hole injection layer for organic light emitting diodes (OLEDs). We found that the adsorption characteristic of HAT-CN on Ca surface is very different from that on Cu surface. HAT-CN is bound to Ca surface strongly through N-Ca bonds, whereas it interacts with Cu surface weakly through physical bonding. Such weak interaction between HAT-CN and Cu surface does not alter the electronic states of HAT-CN, but there is still a charge transfer between them resulting in relative shift of its electronic states to the Fermi level of the interface. On the other hand, due to chemical N-Ca bondings forming at HAT-CN/Ca interface, the electronic states of HAT-CN are significantly modified. Our orbital analysis indicates that orbital mixing readily occurs at the interface resulting in the rearrangements of molecular energy levels, which would enhance the carrier injection in OLEDs.