

## Electronic Structure of Metal/Organic Molecular Film Contacts: Relevance to Carrier Injection - A. Kahn (Princeton University)

Advances in molecular thin-film devices with applications to opto- and microelectronics (light emitting devices, thin film transistors) have been extraordinarily rapid over the past five years. Metal-organic contacts and organic-organic heterojunctions play key roles in the operation of these devices. Efficient injection of charge carriers across interfaces requires increased control of interface chemical and electronic properties. Yet these properties are difficult to determine via standard transport methods because of the complex, and sometime unknown, bulk transport characteristics in these materials. Measurements of interface energetics and chemical structure via direct and inverse photoemission spectroscopy are therefore invaluable for improving our fundamental understanding of these interfaces. This talk describes recent investigations of interfaces between metals (e.g. Al, Mg, Au) and thin films (monolayer to  $\sim 1500\text{\AA}$ ) of  $\pi$ -conjugated molecules (e.g. Alq<sub>3</sub>, F<sub>16</sub>CuPc). The emphasis is placed on the impact of chemical reactions and metal interdiffusion on the carrier injection characteristics at these contacts. We compare metal-on-organic (M/O) interfaces, which are generally broader due to metal interdiffusion into the organic film, with organic-on-metal (O/M) interfaces, where chemical interactions are generally limited to the first molecular plane. The electronic structure of reactive interfaces (e.g. Mg- and Al-Alq<sub>3</sub>, Al-F<sub>16</sub>CuPc) is generally found to be dominated by reaction-induced gap states resulting from the formation of organo-metallic complexes [1]. These reaction-induced states lead to identical positions of the Fermi level and electron and hole barriers at these interfaces, regardless of the deposition sequence. On the other hand, the electronic structure of the non-reactive interfaces (e.g. Au-F<sub>16</sub>CuPc) results from more subtle interactions, which do depend on the deposition sequence. The molecular level alignment at the abrupt O/M interface depends on the work function of the substrate and on the formation of an interface dipole [2], whereas the M/O interface is dominated by doping by isolated metal atoms diffusing into the organic film. These spectroscopy measurements are correlated with current-voltage measurements performed on a number of M/O/M structures, built and tested in ultra-high vacuum.

1. C. Shen, A. Kahn and J. Schwartz, *J. Appl. Phys.* **89**, 449 (2001)
2. C. Shen, A. Kahn and I.G. Hill, in *Conjugated Polymer and Molecular Interfaces*, A. Kahn, J.-J. Pireaux, W.R. Salaneck and K. Seki editors, Marcel Dekker, Inc. (2001).

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