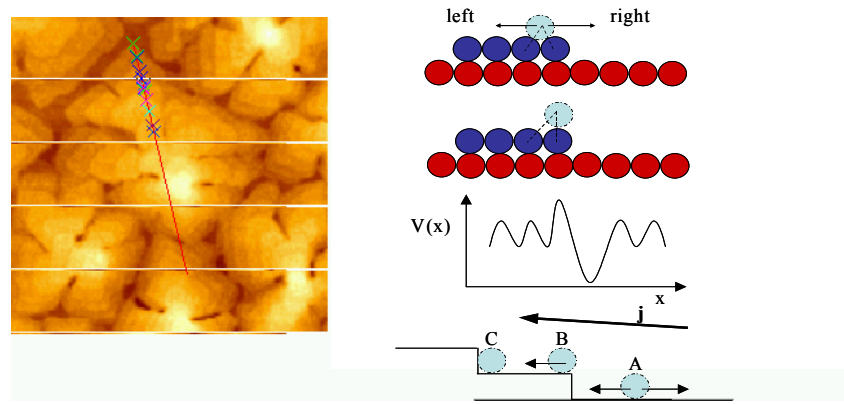
# Interface Characterization of Organic Bistable Devices

Y.Gao, U. Rochester, Y.Yang, UCLA, **DMR-0305111**

•The objective of the project is to understand the interfaces in bistable devices with organic semiconductors as the active component.

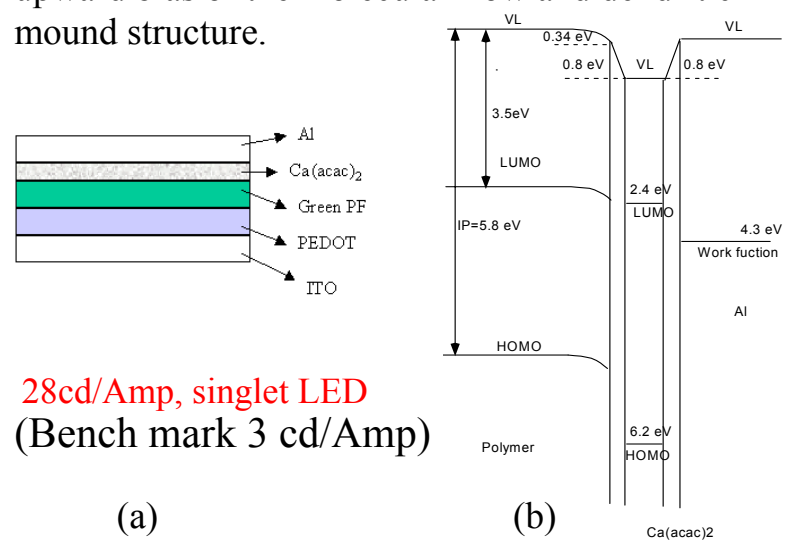
•We studied the growth modes of vacuum evaporated organic thin layers using atomic force microscopy (AFM) and applied dynamic growth theories to explain the observed phenomena. Shown in Fig. 1(a) is the AFM image of pentacene on $SiO_2$, where mound growth is evident that destroys the desirable lateral continuity of the film. Through data analysis and theoretical modeling, we found that the morphology is explained by the existence of Schwoebel barrier, caused by less attraction at the downward step edge, that prevents the molecules from going down the step edge, as shown schematically in Fig. 1(b).

•The knowledge from interface characterization has led us to the fabrication of polymer light-emitting diodes (PLED) of efficiency of 28 cd/Amp, the highest for fluorescence devices. The device is made by inserting ~1 nm thick calcium (2) acetylacetonate [$Ca(acac)_2$] between Al cathode and green emitting polyfluorene (PF), shown Fig. 2(a)). Preliminary energy diagram from interface characterization is shown in Fig. 2(b). The effects of the $Ca(acac)_2$: (1) n-doping of PF that enhances electron injection; (2) perfect LUMO alignment to that of PF for smooth electron transfer; (3) large barrier in HOMO that blocks holes from reaching the cathode without radiative recombination with electrons.




(a) (b)

Fig. 1 (a) The AFM image of pentacene on $SiO_2$. (b) Schwoebel barrier at the step edge that results in the upward bias of the molecular flow and dendritic mound structure.




28cd/Amp, singlet LED
(Bench mark 3 cd/Amp)

(a) (b)

Fig. 2 (a) Schematics of an interface engineered PLED. (b) Energy diagram from interface analysis.

In this project, we investigate the interface properties in model organic bistable devices (OBD) using surface analytical tools. We focus our attention on electronic structures, chemical reactions, interdiffusion, and charge transfer of the organic/metal, organic/organic and organic/dielectric interfaces from a microscopic or atomic viewpoint. The interface characterization includes electronic structure and morphology.

The investigation of the growth of pentacene, one of the most promising organic semiconductors with high charge carrier mobility shows that the growth is a combination of mound growth and diffusion limited aggregation (DLA). Such a combination has not been observed before either experimentally or theoretically. We calculated the height-height correlation functions and obtained effective roughness exponent of about 0.57, and a growth exponent of about 0.27. The former suggests a growth mechanism close to that predicted by non-linear molecular beam epitaxy model, whereas the latter suggests the existence of an instability mechanism caused by mound growth. Our theoretical modeling and computer simulation shows that the formation of discontinuous islands with deep groves are caused by Schwoebel barrier which prevents the molecules from going down the step edge. Such step-bias-induced instability prevents the formation of the much-desired epitaxial growth of pentacene. The fundamental understanding of the growth morphology is crucial for getting high mobility organic thin-film transistors and points to reducing the Schwoebel barrier effect as the route to further improvement of the device performance. The Schwoebel barrier is formed because the attractive interactions a molecule experiences at the downward step are less than that on the terrace. In Fig. 1(c), A, B, and C represents three molecules on the terrace, at the downward step, and at the upward step, respectively. The net flux upward is also marked by the arrow j. Possible means to reduce the effect of the Schwoebel barrer include raising the temperature, improving substrate treatments, and inserting a new interface layer. The latter two methods may only affect the bottom most few molecular layers.

We have demonstrated a very high efficiency green PLED by using a nanoscale interfacial layer to modify the cathode interface. The device structure is Al/Ca(acac)2/polyfluoren/PEDOT/ITO. The luminescence efficiency achieved was as high as 28 cd/A, the highest efficiency ever achieved in fluorescence singlet devices, including both OLEDs and PLEDs. The $Ca(acac)_2$ layer inserted between the emitting polymer layer and Al electrode plays multifunctional roles, as shown in the energy diagram from interface characterization: (a) it reduces the electron injection barrier height by n-doping of PF; (b) it has a perfect alignment of the lowest unoccupied molecular orbital (LUMO) with that of PF, resulting in a smooth electron transfer; (c) it behaves as a hole-blocking layer because of the large barrier in highest occupied molecular orbital (HOMO) from that of PF, that subsequently blocks holes from reaching the cathode without radiative recombination and helps the injection of electrons by Coulomb attraction force. Furthermore, it also prevents the quench of luminescence by the cathode. As a result, the efficiency of our green devices was improved dramatically. We are currently performing further interface characterization studies to evaluate each contributing factor. In comparison, the efficiency of Ca/polyfluoren/PEDOT/ITO device is 9 cd/A, and the bench mark value for high efficiency is 3 cd/A from Alq/NPB devices.

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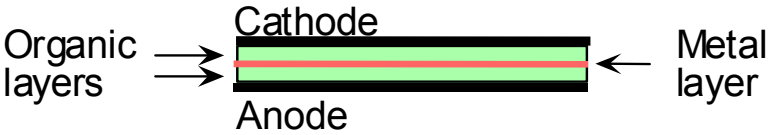


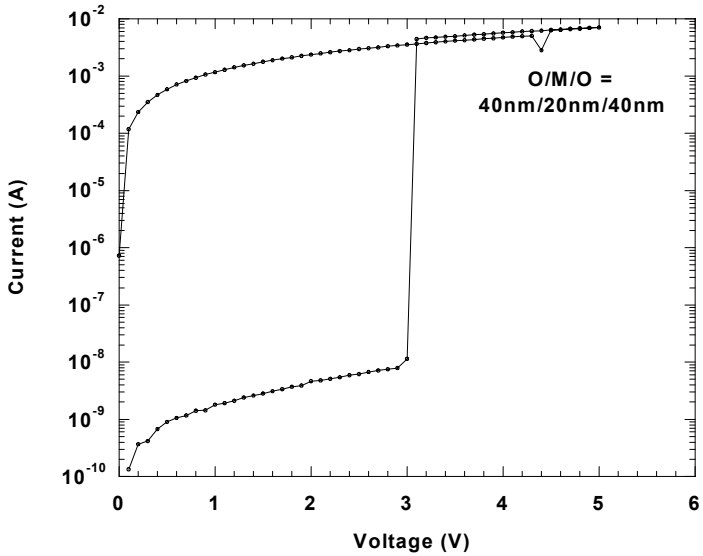


- Metal insertion mid-layer produces pronounced current bistability of ratio~$10^6$
- Interface characterization critical for understanding the mechanism
- Thickness and morphology of the metal mid-layer and organic materials are important.

Electrical bistability is a novel phenomenon in which the device shows two distinctively different resistivities at the same bias voltage in a specific voltage range. Previously observed electrical bistable behavior mainly involves metal-insulator transition in inorganic semiconductors at cryogenic temperatures and as a result, is limited in practical applications. Recently, one of us (YY) discovered that organic thin-film devices show remarkably bistability at room temperature (L.P. Ma, J. Liu, and Y. Yang, Appl. Phys. Lett. **80**, 2997 (2002)). The device is made by inserting a thin metal mid-layer (~20 nm) in an organic semiconductor layers sandwiched between metal electrodes. Upon scanning up the biasing voltage (I-V measurement), the injection current could be "switched-upward" by several orders of magnitude at a threshold voltage, typically +3V. Once swithced-up, the device remain highly conductive even at biases below the threshold voltage, and the low conductivity state can only be recovered by a high reverse bias ~ –5V. The organic bistability is nonvolatile, i.e. it remains in either of the two (high or low conductivity) states at the time when the bias is removed for days. The magnitude of the bistability is the highest ever been reported in the literature, and it occurs at room temperature. It's therefore clear that the OBD can be controlled, this device will be a promising candidate for nonvolatile memory applications. This behavior is ideal for electronic memory cells and switches.

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## Education:

Two graduate students (Serkan Zorba (UR) and Faye Xu (UCLA)) have made significant contributions in the project. Serkan is particularly experienced in scanning probe microscopy and organic thin film morphology, and developed theoretical modeling and simulation to explain the observed morphology. Faye has participated in the fabrication of a large number of different organic devices, and recently demonstrated the highest quantum efficiency polymer LEDs due to the nano-scale interface engineering. In addition, we have hosted Steward Knox (UR) as part of the REU program.

## Outreach:

In collaboration with Barb King, we are making progress in enhancing the science education program in Cobblestone school, a private school with pre-K to 10$^{th}$ grade programs in Rochester, NY. In the picture, Y.G. is demonstration to the pre-K class convection and the motion of interface.