

Combined photoemission/*in vacuo* transport study of the indium tin oxide/copper phthalocyanine/*N,N'*-diphenyl-*N,N'*-bis(*l*-naphthyl)-1,1'-biphenyl-4,4''diamine molecular organic semiconductor system

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Ultraviolet photoemission spectroscopy (UPS) was used to study the indium tin oxide/copper phthalocyanine (CuPc) and CuPc/*N,N'*-diphenyl-*N,N'*-bis(*l*-naphthyl)-1,1'-biphenyl-4,4''diamine interfaces, which are commonly used as an anode/hole injection layer/hole transport layer combination in organic light emitting devices. In order to assess the validity of the transport barriers measured using UPS, *in vacuo* *I-V* measurements have been performed on simple devices grown and measured in the same system as the samples studied using UPS. *I-V* characteristics were modeled using numerical simulations. The parameters used in the simulated curves which best fit the measured *I-V* characteristics agree quantitatively with the UPS measured barriers. © 1999 American Institute of Physics. [S0021-8979(99)04716-7]

INTRODUCTION

Small-molecule based organic light emitting devices (OLEDs) have been the focus of much research in recent years.¹ Great improvements in device quantum efficiencies have been realized, but in order to further improve the power efficiency it is desirable to decrease the required drive voltages. High drive voltages are the result of several factors, including poor carrier mobilities, and large carrier injection barriers at metal/organic and organic/organic interfaces. The analysis of one method of improving charge injection is described in this article.

A thin layer of copper phthalocyanine (CuPc) between the transparent anode, indium tin oxide (ITO) coated glass, and a hole transporting material, such as *N,N'*-diphenyl-*N,N'*-bis(*l*-naphthyl)-1,1'-biphenyl-4,4''diamine (α -NPD) or the closely related material *N,N'*-diphenyl-*N,N'*-bis(3-methylphenyl)-[1,1'-biphenyl]-4,4''diamine (TPD), is widely used to improve hole injection into OLEDs.²⁻⁶ While the exact mechanism for the resulting decrease in device turn-on voltage is not understood, the relative energies of the organic molecular levels estimated assuming vacuum level alignment at all interfaces places the CuPc highest occupied molecular orbital (HOMO) between the ITO Fermi level and the α -NPD (or TPD) HOMO.^{4,6} It has therefore been suggested that the resulting staircase arrangement of hole transporting molecular levels must improve charge transport. While this suggestion may seem reasonable, the mechanism for improving injection is still not obvious, as a hole originating from the Fermi level within the ITO must still overcome two barriers, the sum of which is equal to the barrier which would be encountered at the ITO/ α -NPD (TPD) interface if the CuPc layer were absent. Simple statistical arguments, based on thermal equilibrium, would lead one to conclude that the probability of an indi-

vidual carrier being excited over both barriers should be equal to that of a carrier being excited over a single barrier equal to the sum of the two smaller barriers.

We have studied this multilayer system with combined ultraviolet photoemission spectroscopy (UPS) and *in vacuo* *I-V* measurements. UPS allows precise measurement of the energetic positions of the organic HOMO levels at the heterointerfaces, and *I-V* measurements of simple hole-only devices allow the transport characteristics of the structure to be examined directly, without the contributions of electron transport and exciton recombination which are present in full OLED devices. Additionally, while most UPS studies are performed under UHV conditions on samples grown in UHV, most OLEDs are grown at 10^{-6} – 10^{-5} Torr, and *I-V* measurements are typically performed in air, or at atmospheric pressure in the controlled atmosphere of a glove box. These extreme differences in sample preparation may lead to thin films and interfaces of differing electronic character. In the current study, we have eliminated these sources of uncertainty by fabricating and testing devices under the same conditions as the samples studied using UPS.

EXPERIMENT

ITO substrates (Applied Films Corp. $\approx 20 \Omega/\square$) were prepared by cleaning in boiling trichloroethylene, acetone, and boiling methanol prior to being introduced into the vacuum system. No further treatment was applied. The source of the ITO, and the pretreatments used, can strongly affect the work function of the ITO surface, and therefore the hole injection barrier. Nüesch *et al.*⁷ have recently found that the work function of ITO can be varied from 3.9 to 5.1 eV by dipping the ITO in acids or bases prior to loading the substrates into vacuum.

The depositions described later, as well as the *I-V* measurements, were performed at $\approx 1 \times 10^{-9}$ Torr. The UPS measurements were performed in an analysis chamber (base pressure $\approx 4 \times 10^{-11}$ Torr) connected to the growth chamber,

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using a He discharge lamp, and a double-pass cylindrical mirror analyzer. The resolution of the measurements was ≈ 150 meV, as determined from the width of the Fermi edge of freshly deposited Au. All evaporations were performed from heated effusion cells and calibrated using a quartz crystal microbalance.

UPS spectra of the clean ITO surfaces were studied to determine the energy of the valence band maxima and vacuum levels relative to the Fermi level. A thin layer of CuPc (typically 4 Å) was deposited, and UPS spectra were collected. This process was repeated, doubling the total CuPc thickness at each step, until the UPS spectra were representative of a clean CuPc surface, and the ITO features were suppressed. The spectra were examined for evidence of band bending and interface dipoles as a function of CuPc thickness. After correcting for band bending, if present, the position of the top of the CuPc HOMO at the interface was determined relative to the Fermi level. We define the UPS hole barrier, ϕ_{UPS} , as the energy difference between the Fermi level and the zero crossing of the linear extrapolation of the low binding energy edge of the organic HOMO.

The second interface, that between CuPc and α -NPD, was studied as described earlier for incremental deposition of α -NPD on a 100-Å-thick layer of CuPc. The positions of the CuPc and α -NPD HOMOs at the interface were determined relative to the Fermi level. The difference between the α -NPD and CuPc HOMO positions at the interface represents the barrier to hole injection from CuPc to α -NPD. For comparison, the interface between ITO and α -NPD was also studied, and the hole injection barrier from ITO into α -NPD was determined.

Simple device structures were grown in the same vacuum system, under the same conditions as the samples studied by UPS, with the exception of an increased deposition rate ($1\text{--}4 \text{ \AA s}^{-1}$ compared to $0.1\text{--}0.2 \text{ \AA s}^{-1}$). Two structures were considered: ITO:35 Å CuPc:1200 Å α -NPD:500 Å Al, and ITO:1200 Å α -NPD:500 Å Al. The electron injection barrier from Al into α -NPD is much larger than the hole injection barrier from ITO into α -NPD, as estimated from previous systematic studies of the metal/ α -NPD hole injection barrier as a function of metal work function.⁸ We therefore expect the current in these devices to be predominantly due to hole transport. Assuming a density of 1.7 g cm^{-3} for CuPc, the thickness of the CuPc layer was estimated to be $35 \pm 5 \text{ \AA}$. The sticking coefficients were assumed to be equal to unity for all depositions.

RESULTS

The results of the UPS study of the ITO/CuPc interface are presented in Fig. 1. The bottom spectrum contains the broad, featureless, characteristics of clean ITO. The CuPc HOMO (at ≈ -1.5 eV) is first visible at a thickness of $\approx 4 \text{ \AA}$, and increases in intensity with increasing thickness. The binding energies of the CuPc spectral features do not change with increasing thickness, indicating a flat-band condition on the length scale of the film thickness studied here.

There is no systematic shift in the vacuum level (seen from the onset of photoemission on the high binding energy

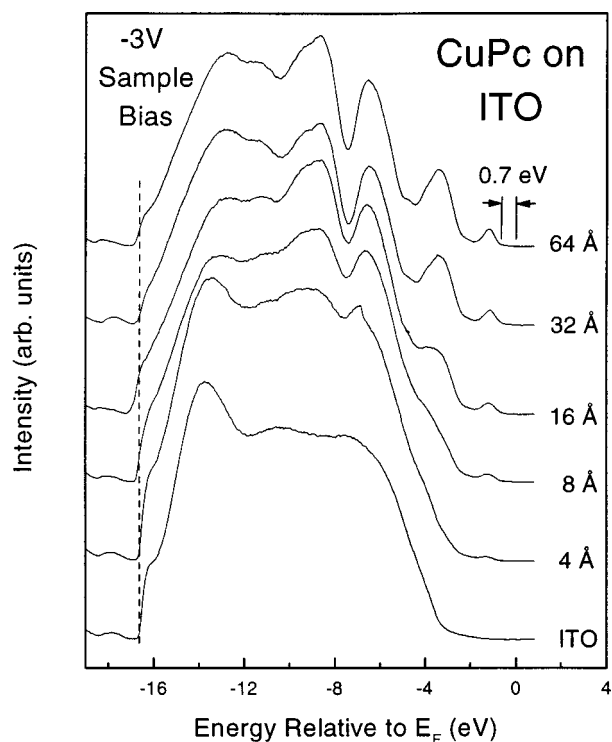


FIG. 1. He I (21.22 eV) UPS spectra of CuPc on ITO. 0.7 eV represents the offset between the Fermi level (E_F) and the low binding energy edge of the CuPc HOMO.

side of the spectra), indicating an alignment of the vacuum levels of the materials at the interface, within our experimental uncertainty of ± 100 meV. The offset between the Fermi level (E_F) and the top edge of the CuPc HOMO, which represents the barrier to hole injection from the ITO, is measured to be 700 ± 100 meV. Lee *et al.*⁹ have reported a slightly larger barrier (1.0 eV), but as noted in the Experiment section, the ITO work function depends strongly on the preparation procedures.

The UPS data from the CuPc/ α -NPD interface are presented in Figs. 2 and 3. The bottom spectrum is characteristic of a saturated CuPc surface. The deposition of α -NPD, on this surface results in an interface which can be well approximated using vacuum level alignment, as has been reported elsewhere.¹⁰ There is no evidence of band bending in either layer, as the binding energies of all spectral features remain constant as a function of α -NPD coverage. A saturated α -NPD spectrum is not observed, however, until a nominal thickness of 96 Å is reached, which is much larger than the UPS probing depth of $\approx 10\text{--}15 \text{ \AA}$. This may indicate that the α -NPD has a low sticking probability on the CuPc surface, or that it undergoes three dimensional island growth, leading to incomplete coverage until these islands coalesce. The CuPc and α -NPD HOMOs are well separated, and clearly resolved, as can be seen in Fig. 3. The difference in binding energies of the two HOMO edges, which represents the barrier to hole transport from CuPc to α -NPD, is 500 ± 100 meV. This result, which we have reported earlier,¹⁰ has recently been verified by Lee *et al.*⁹ who measured this barrier to be 0.4 eV.

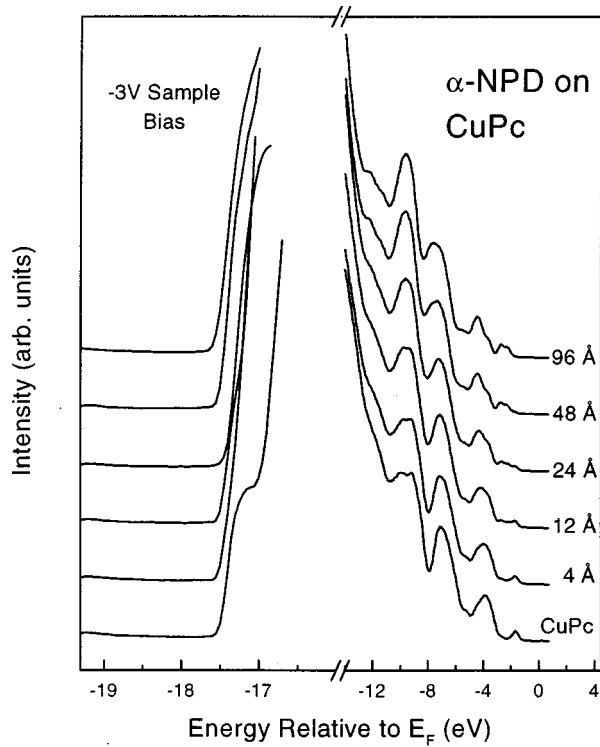


FIG. 2. UPS data for the interface formed by depositing α -NPD on CuPc.

The $I-V$ characteristics of the simple device structures are presented in Fig. 4. The ITO: α -NPD:Al device $I-V$ characteristics are assumed to be contact limited, due to the large (≈ 1.2 eV, Fig. 5) hole injection barrier at the untreated ITO/ α -NPD interface. Enhanced hole injection is evident in the ITO:CuPc: α -NPD device. The measured current in these devices exceeds that of the α -NPD-only devices over the entire range for which the currents exceed the noise level. At an average electric field of 1.2×10^6 V/cm, the current en-

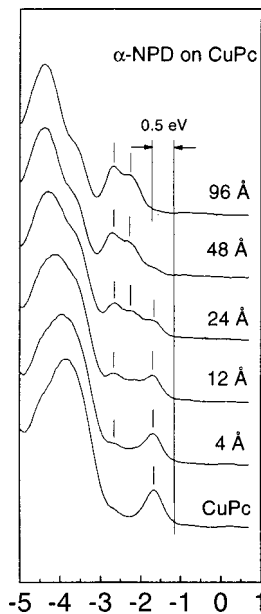


FIG. 3. Close up of the HOMO region of the data in Fig. 2. 0.5 eV is the measured barrier for hole injection from CuPc into α -NPD.

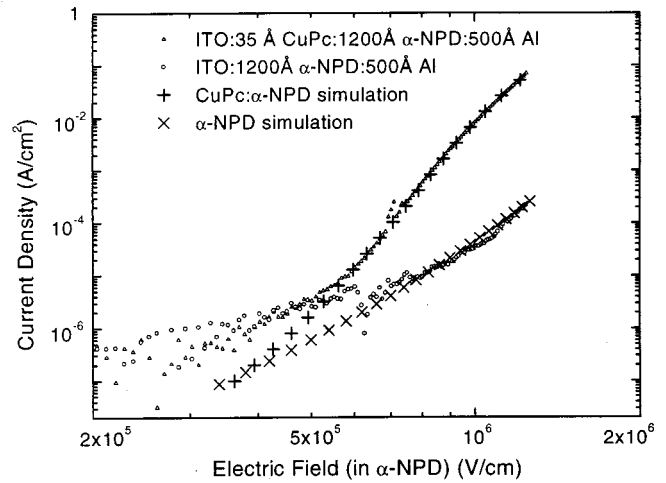


FIG. 4. *In vacuo* $I-V$ characteristics of simple diode structures. The enhanced hole injection resulting from the thin CuPc layer is evident.

hancement is $\approx 10^3$. This further supports the assumption of contact limited currents in the α -NPD-only devices, as one would not expect such a marked increase in the current upon modifying the contact region if transport in the α -NPD were bulk limited.

DISCUSSION

The UPS data presented above can be used to construct the molecular level alignment diagrams presented in Fig. 6. The linear extrapolation of the low binding energy edge of the HOMO to zero intensity is based on a method used for inorganic semiconductors to determine the position of the

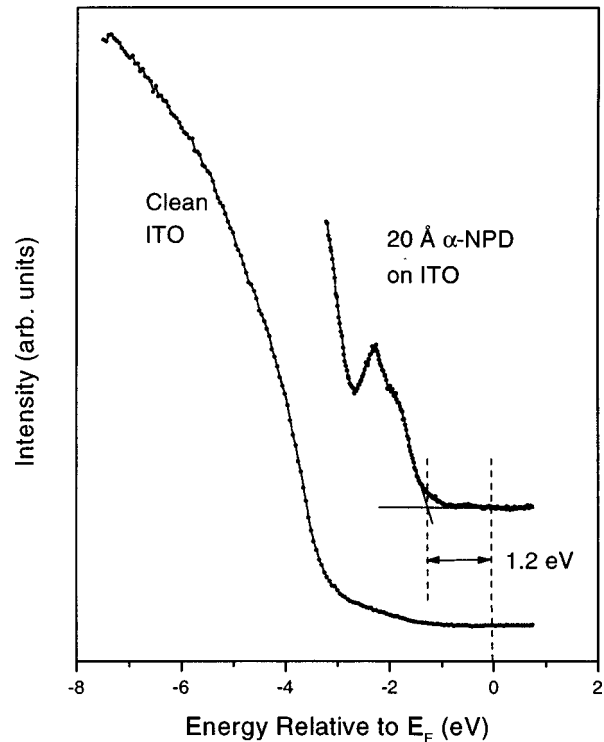


FIG. 5. UPS data for the interface between ITO and α -NPD.

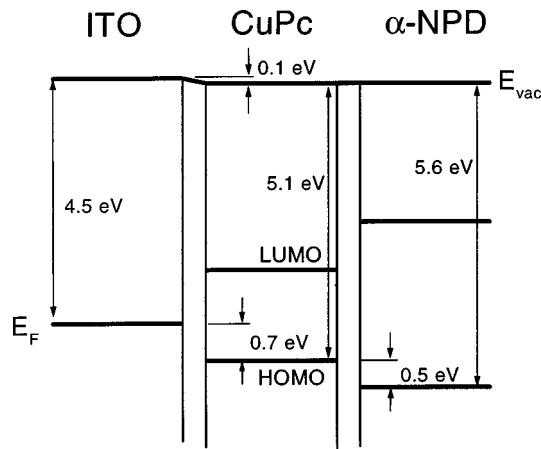


FIG. 6. Molecular level alignment diagrams constructed using the HOMO and vacuum levels measured using UPS. The lowest unoccupied molecular orbital (LUMO) positions are inferred assuming a HOMO/LUMO gap equal to the onset of optical absorption.

top of the valence band. In the case of inorganics, this method is known to be reasonably accurate when compared to models of the density of states in the vicinity of the valence band maximum. In the present case, that of a randomly disordered organic semiconductor, this method is used by convention, and has not been justified on any physical basis. This convention is useful when comparing relative barriers between different metals and the same organic, for instance, where the change in barrier height with the metal work function will be accurately determined. However, the magnitude of an individual barrier may not be correct.

Transport through the ITO:CuPc: α -NPD:Al devices was simulated numerically, to correlate the UPS and $I-V$ measurements. The HOMO was simulated as a finite number of states ($1.5 \times 10^{21} \text{ cm}^{-3}$) at a single energy (the density of states was approximated by a delta function). This state will be referred to as the isoelectronic transport level, after Campbell *et al.*¹¹ The following assumptions were used in the simulations: (1) the structures were treated as hole-only devices, (2) thermodynamic equilibrium was assumed to be maintained at the ITO/CuPc interface,^{16,12} (3) thermodynamic equilibrium was assumed to hold at the CuPc/ α -NPD interface, (4) the Einstein relation was assumed to be valid, such that $D = \mu kT/q$, and (5) the mobility, μ , was assumed to be independent of the electric field. The current in the α -NPD layer was assumed to be determined by the hole den-

sity in the α -NPD and the electric field at the interface (the diffusion current in the α -NPD layer is neglected). The drift/diffusion equation,

$$q\mu n(x)E(x) - qD \frac{dn}{dx} - j = 0, \quad (1)$$

$$\epsilon \frac{dE}{dx} = qn(x), \quad (2)$$

was solved numerically within the CuPc layer using the equilibrium charge density at the ITO/CuPc interface, including image force barrier lowering, and the current in the α -NPD layer as boundary conditions. It should be noted that these equations implicitly include the effects of space charge, and space-charge limited conduction is simply the solution of these equations in the limit of small hole injection barriers.

The simplified transport equations given earlier can be justified on the following grounds: (1) The effect of traps are not included, as previous studies have found that hole transport in α -NPD is trap-free.^{13,14} (2) The field dependence of the α -NPD hole mobility is very weak.¹⁵ In fact, the hole mobility only changes by a factor of ≈ 1.7 over the range of electric fields for which the simulated data is presented. This is negligible compared to the increase in current by six orders of magnitude over the same range of electric fields. (3) The assumption of thermodynamic equilibrium at the ITO/CuPc interface has previously been verified by Davids, Campbell, and Smith.¹⁶ Equilibrium is the result of strong hole scattering near the interface, and the low mobility of the carriers.

The results of this calculation are included in Fig. 4, and the parameters used in the calculation are presented in Table I. The agreement between the experimental and calculated $I-V$ characteristics is extremely good over the entire experimentally accessible range, which spans 5 orders of magnitude in current. Also included in Fig. 4 are the experimental data and calculated $I-V$ characteristics for the α -NPD-only devices. The calculations assume thermodynamic equilibrium at the ITO/ α -NPD interface and image force lowering of the barrier. A constant mobility of $1 \times 10^{-3} \text{ cm}^2/\text{Vs}$ and a relative permittivity of 1.5 were assumed for the organic layer.

In order to understand the transport of holes within the ITO/CuPc/ α -NPD devices, the low and high field limits will be discussed. At zero electric field (and assuming that the built-in potential is zero), the charge density within the

TABLE I. Parameters measured using UPS, corrected UPS parameters which can be compared with the simulated parameters, and parameters used in the transport simulations.

	ITO/CuPc barrier (eV)	CuPc/ α -NPD barrier (eV)	L_{CuPc} (\AA)	$\epsilon_{\tau, \text{CuPc}}$	$\epsilon_{\tau, \alpha\text{-NPD}}$	μ_{CuPc} cm^2/Vs	$m\mu_{\alpha\text{-NPD}}$ cm^2/Vs
UPS	0.7 ± 0.1	0.5 ± 0.1	35
Corrected	0.46 ± 0.08	0.43 ± 0.1^a 0.26 ± 0.1^b
Simulation	0.51	0.40^a 0.20^b	30	3	1.5	10^{-3}	10^{-3}

^aLow-field limit.

^bHigh-field limit.

α -NPD at the interface with CuPc is simply given by the density of states in the α -NPD times the Boltzmann factor evaluated at the isoelectronic HOMO level, which is at an energy equal to $\phi_{\text{ITO/CuPc}} + \phi_{\text{CuPc}/\alpha\text{-NPD}}$ away from the Fermi energy. Therefore, at very small electric fields, injection into the device is similar to that which would be expected if an organic with a hole injection barrier equal to the sum of the two barriers was in direct contact with the ITO. The magnitude of the above sum is $\approx 1.2 \pm 0.14$ eV, as measured by UPS, which is in agreement with the measured barrier of 1.2 ± 0.1 eV for α -NPD on untreated ITO (Fig. 5).

At high electric fields, a large amount of charge is injected into the CuPc layer, but blocked at the CuPc/ α -NPD interface. This is a result of the image force lowering of the ITO/CuPc barrier. At 5×10^6 V/cm, the ITO/CuPc barrier is reduced by ≈ 0.5 eV, and is therefore smaller than the CuPc/ α -NPD barrier. This results in an accumulation of charge at the interface, a large charge density gradient within the CuPc layer, and thus a large diffusion current flowing back to the ITO contact which almost cancels the forward flowing drift current. This accumulation of charge at the interface implies that the quasi-Fermi level will move towards the CuPc HOMO. Its position can be calculated from the accumulated charge density. The distance between the quasi-Fermi level and the α -NPD HOMO is correspondingly reduced, and the charge density within the α -NPD is given by the Boltzmann factor evaluated at $\phi_{\text{CuPc}/\alpha\text{-NPD}}$ times the charge density within the CuPc layer at the interface. We therefore expect that at high fields the current will be limited by the CuPc/ α -NPD barrier. In fact, if the accumulated charge density was to approach the density of states in the CuPc, or equivalently the quasi-Fermi level was to reach the isoelectronic CuPc HOMO, the I - V characteristics above this field should be the same as that of a device in which an organic with a hole injection barrier equal to the CuPc/ α -NPD barrier was directly in contact with the ITO, and completely independent of the CuPc/ITO injection barrier. This current is much larger than the low-field limiting case, because of the relative sizes of the barriers. The high and low-field limits are illustrated in Fig. 7.

Between the high- and low-field limits, there must exist a transition, where the current increases rapidly with applied bias as holes accumulate at the CuPc/ α -NPD interface. It is this transition which dominates the measured I - V characteristics presented in Fig. 4.

It should be noted that a recent study by Aziz *et al.*¹⁷ found that including a CuPc buffer layer actually decreased hole injection in their devices. For the CuPc layer to improve injection the CuPc/ α -NPD barrier must be smaller than the ITO/ α -NPD barrier. If this is not the case, the current in the high-field limit will be smaller than that in the α -NPD-only devices at the same bias. The work function of the ITO being used will therefore determine whether the CuPc interlayer improves or degrades hole injection. As noted earlier, the work function of ITO has been found to depend strongly on the preparation procedure used prior to organic deposition.⁷

Support for our model can also be found in a recent study of Giebeler *et al.*,¹⁸ who reported that inserting a layer of starburst amine (*m*-MTDATA) between ITO and α -NPD

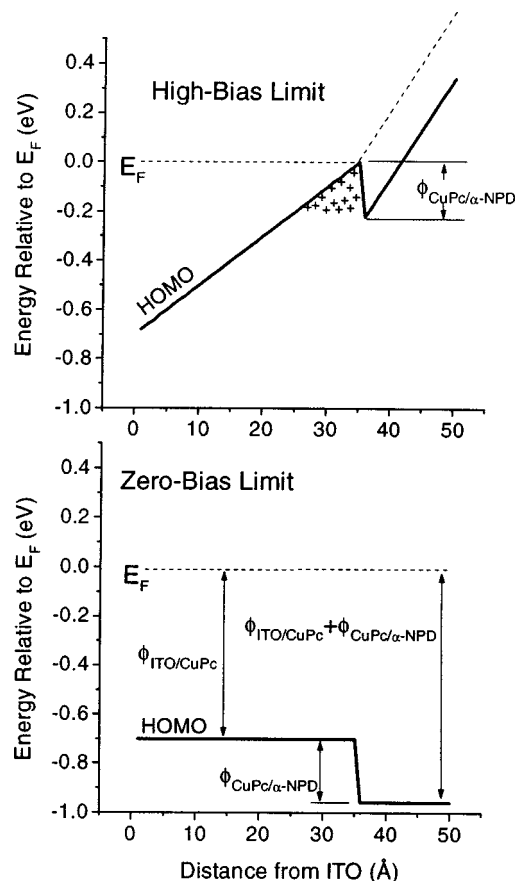


FIG. 7. High- and low-field limits of the ITO/CuPc/ α -NPD system. At low fields, injection is limited by the sum of the two barriers, while at high fields it is limited by the CuPc/ α -NPD barrier.

improved hole injection. As in our ITO/CuPc/ α -NPD system, the HOMO of the interlayer material (*m*-MTDATA) is at an intermediate energy, between the ITO Fermi level and the α -NPD HOMO, and thus the mechanism for improved hole injection is the same.

Although the agreement between the calculated and experimentally determined I - V curves is extremely good, the barriers used in the ITO/CuPc/ α -NPD and ITO/ α -NPD simulations are significantly smaller than those measured by UPS (Table I). To address this discrepancy, we must reconsider the arbitrary convention of determining the low-binding energy cut-off of the HOMO from the zero crossing of the linear extrapolation of the spectroscopic HOMO peak.

The UPS measured density of states of a single molecular level is closely approximated by a Gaussian peak. The spectral peaks are much broader than the instrumental resolution. This shape is therefore related to the actual density of states. Indeed, energetic models of the bulk density of states often use a Gaussian distribution to reflect the random energetic disorder, caused by inequivalent molecular coordination in these amorphous materials,¹⁹ which is further broadened by thermal excitation and the superposition of bulk and surface components in the UPS spectra.²⁰

In most models of injection and transport, the transport level (HOMO for holes), is assumed to consist of a finite density of states at a single energy level. Furthermore, the occupation of these states is usually described using Boltz-

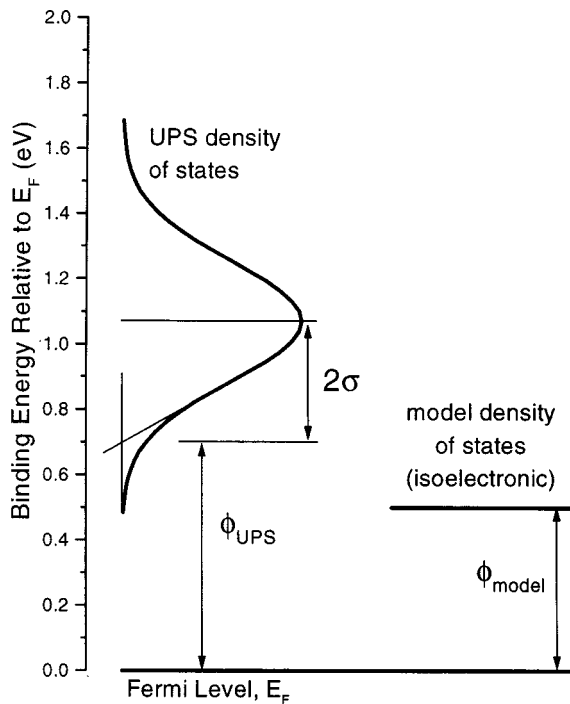


FIG. 8. UPS (Gaussian) and model (isoelectronic) densities of states, and the corresponding definitions of the injection barriers.

mann statistics, which is valid for Fermi level positions more than a few kT away from the transport level. If we are to compare real $I-V$ data with such models, we must examine the relationship between the barriers measured using UPS, ϕ_{UPS} , and the barriers used in these isoelectronic transport models, ϕ_{model} . The two models of the density of states, Gaussian and isoelectronic, are shown schematically in Fig. 8.

For a Gaussian distribution, the linear extrapolation from the point of inflection on one side of the peak can be shown to cross zero at a point which is 2σ from the peak maximum, where σ is the standard deviation of the distribution. In order to achieve the same total charge density in the Gaussian distribution and the discrete model transport level (assuming the same total number of states in each), the following relationship between ϕ_{UPS} and ϕ_{model} must be true,

$$FD(\phi_{model}) \approx e^{-\phi_{model}/kT} = \int_{-\infty}^{\infty} \frac{FD(E)}{\sigma\sqrt{2\pi}} e^{-(E-(\phi_{UPS}+2\sigma))^2/2\sigma^2} dE, \quad (3)$$

where $FD(E)$ is the Fermi-Dirac distribution function, and the Fermi energy has been chosen as zero for the energy scale. Solving for the appropriate value of ϕ_{model} as a function of ϕ_{UPS} ,

$$\phi_{model} = kT \ln \left[\left(\int_{-\infty}^{\infty} \frac{FD(E)}{\sigma\sqrt{2\pi}} \times e^{-(E-(\phi_{UPS}+2\sigma))^2/2\sigma^2} dE \right)^{-1} - 1 \right], \quad (4)$$

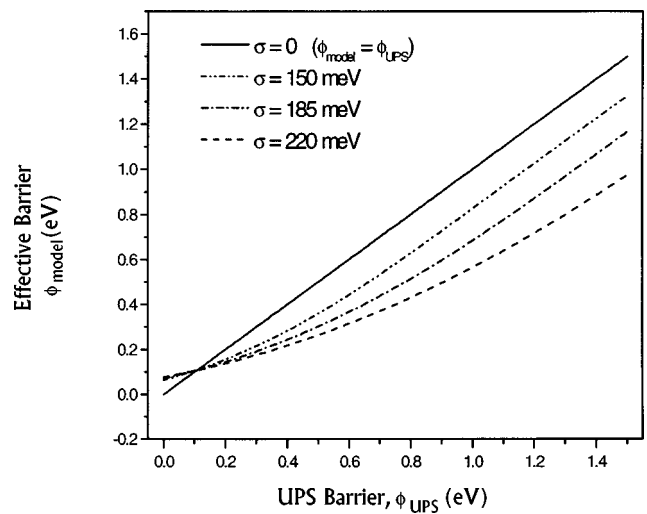


FIG. 9. Relationship between the UPS measured barrier, ϕ_{UPS} , and the appropriate barrier to be used in isoelectronic transport level modeling, ϕ_{model} . The four curves are for $\sigma=0$ (isoelectronic), 0.15, 0.185, and 0.22 eV.

where Fermi-Dirac statistics have been used throughout such that ϕ_{model} and ϕ_{UPS} can be compared for all values. Figure 9 shows the relationship between ϕ_{UPS} and ϕ_{model} for $\sigma=0, 150, 185,$ and 220 meV, the first corresponding to $\phi_{model}=\phi_{UPS}$, and the last three spanning the range of organic peak widths typically seen in UPS studies. Note that ϕ_{model} is significantly smaller than ϕ_{UPS} for all values of $\phi_{UPS} \geq 100$ meV. Model barriers calculated in this way will be also be referred to as ‘‘corrected’’ UPS barriers.

Within the scope of this simple model, injection at metal/organic interfaces is straightforward. Given measured values of ϕ_{UPS} and σ , a value of ϕ_{model} can be computed and compared with numerical simulations. However, the situation is somewhat more complicated at organic-organic heterointerfaces. The barrier to hole injection is given by $\phi_{UPS,2} - \phi_{UPS,1}$, where holes flow from organic 1 into organic 2. Under bias, holes will accumulate at an interface with a positive barrier. This accumulation, and therefore the position of the hole quasi-Fermi level at the interface, will strongly depend on the applied bias. As the Fermi level shifts towards the HOMO, the values of $\phi_{UPS,1}$ and $\phi_{UPS,2}$ are each decreased by the magnitude of the shift. The barrier which must be used in an isoelectronic model to insure thermodynamic equilibrium at the heterointerface is given by $\phi_{model,2} - \phi_{model,1}$. Because the derivative, $d\phi_{model}/d\phi_{UPS}$, decreases with decreasing ϕ_{UPS} , $\phi_{model,1}$ will decrease more slowly than $\phi_{model,2}$, and the model heterointerface barrier will decrease with increasing hole accumulation at the interface.

Nonlinear least squares fitting was used to determine the widths of the UPS HOMO peaks. The widths of the CuPc and α -NPD HOMO peaks were found to be very similar, and $\sigma=0.185$ eV was used to calculate the effective model barriers. The ITO/CuPc UPS barrier was measured to be 0.7 ± 0.1 eV, and the corresponding corrected value is 0.46 ± 0.08 eV which agrees well with the value of 0.51 eV which was used in the simulation. The corrected CuPc/ α -NPD het-

erojunction UPS barrier was calculated for two situations: the low-field limit (at zero applied bias), and the high-field limit, corresponding to the highest simulated field presented in Fig. 4. The low-field barrier, calculated from the UPS measured peak positions is 0.43 ± 0.1 eV, and the simulated $I-V$ curve was calculated using a low-field barrier of 0.40 eV. The high-field barrier calculated from the UPS data is 0.26 ± 0.1 eV, and the simulated value is 0.20 eV.

In the case of the α -NPD-only devices, a zero-field effective barrier height of 0.87 eV was used. This is in excellent agreement with the corrected UPS barrier of 0.9 ± 0.1 eV, which was calculated from the measured UPS barrier, ϕ_{UPS} of 1.2 ± 0.1 eV.

CONCLUSION

The ITO CuPc/ α -NPD organic semiconductor multilayer system was investigated using UPS and *in vacuo* $I-V$ measurements. A model of the hole transport in this system was developed which accurately reproduces the measured $I-V$ characteristics using parameters which are in quantitative agreement with the transport barriers measured using UPS. This agreement was only achieved after the shape of the HOMO density of states was taken into account, and the injection barriers used in the simulations adjusted accordingly. This effect must be taken into account when interpreting UPS data, and particularly when evaluating barriers between two organics, or comparing barriers between metals and different organics, where the different HOMO peak widths of dissimilar organics may significantly impact a comparison of the relative barriers.

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