Deep Blue/Ultraviolet Microcavity OLEDs

Based on Solution-Processed PVK:CBP Blends

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There is an increasing need to develop stable, high-intensity, efficient OLEDs in the deep blue and UV. Applications include blue pixels for displays and tunable narrow solid-state UV sources for sensing, diagnostics, and development of a wide band spectrometer-on-a-chip. With the aim of developing such OLEDs we demonstrate an array of deep blue to near UV tunable microcavity (μc) OLEDs ($\lambda \sim 373\text{--}469\text{ nm}$) using, in a *unique* approach, a mixed emitting layer (EML) of poly(*N*-vinyl carbazole) (PVK) and 4,4'-bis(9-carbazolyl)-biphenyl (CBP), whose ITO-based devices show a broad electroluminescence (EL) in the wavelength range of interest. This 373–469 nm band expands the 493–640 nm range previously attained with μc OLEDs into the desired deep blue-to-near UV range. Moreover, the current work highlights interesting

characteristics of the complexity of mixed EML emission in combinatorial 2-d μ OLED arrays of the structure 40 nm Ag/ x nm MoO_{*x*}/~30 nm PVK:CBP (3:1 weight ratio)/ y nm 4,7-diphenyl-1,10-phenanthroline (BPhen)/1 nm LiF/100 nm Al, where x = 5, 10, 15, and 20 nm and y = 10, 15, 20, and 30 nm. In the short wavelength μ c devices, only CBP emission was observed, while in the long wavelength μ c devices the emission from both PVK and CBP was evident. To understand this behavior simulations based on the scattering matrix method, were performed. The source profile of the EML was extracted from the measured EL of ITO-based devices. The calculated μ c spectra indeed indicated that in the thinner, short wavelength devices the emission is primarily from CBP; in the thicker devices both CBP and PVK contribute to the EL. This situation is due to the effect of the optical cavity length on the relative contributions of PVK and CBP EL through a change in the wavelength-dependent emission rate, which was not suggested previously. Structural analysis of the EML and the preceding MoO_{*x*} layer complemented the data analysis.

1. Introduction

OLEDs are being increasingly used for display and solid state lighting technologies. They are also attractive for analytical applications, advancing development of compact sensors and on-chip spectrometers [1-15]. However, there exists a need for improvement in deep blue OLEDs for lighting and displays and UV OLEDs as excitation sources in sensing and analytical applications. Particularly of interest for analytical applications are narrow-band multi-color microcavity (μc) OLED arrays, which can be used in on-chip spectrometers or in multianalyte chemical or biological sensing [1,2,16,17]. Although there have been studies on novel UV emitters, these studies focused solely on non- μc , ITO-based devices with broad electroluminescence (EL) bands [18-21]. Other UV sources have often relied on bulky, environmentally unfriendly discharge lamps. There is an increasing need to develop compact solid-state UV sources also for other applications such as germicidal disinfection, UV water treatment, sterilizing surfaces in industrial and medical environments, treatment of skin conditions such as psoriasis, and developing anti-counterfeiting signatures for forensic applications [22]. Many of these applications would greatly benefit from tunable compact, portable hand-held LED or OLED based sources.

Tunable OLED and μc OLED arrays with band emission from blue to red wavelengths have been previously studied using various techniques, including doped-layer thickness variation and grayscale lithography that resulted in an array with peak emissions in the range of 472 to 606 nm [2,23]. Recently, Liu et al. incorporated a simple method of hole injection layer-thickness-variation using various thicknesses of molybdenum oxide (MoO_x) to generate a μc array with peak emissions in the range of 493 to 640 nm [16]. To generate arrays of multi-color μc OLEDs a broad-band-based emission of the analogous ITO-based devices is required. That is, the EL of

the ITO-based devices should be broad enough to cover the wavelengths desired for the μ OLEDs. In this way, high quality, narrow peaks can be obtained across a range of wavelengths. Herein we present a *unique* approach for multi-colored μ OLED arrays in the deep blue and UV. Mixing the polymer poly(*N*-vinyl carbazole) (PVK) with the small molecule 4,4'-bis(9-carbazolyl)-biphenyl (CBP) results in a combined emission that is broad across the near UV and blue regions (373 – 469 nm). This development brings us closer to an on-chip spectrometer that covers a wider spectral range. Moreover, the work highlights interesting fundamental characteristics of the complexity of mixed emitting layer (EML) emission in 2-d combinatorial μ OLED arrays, particularly in devices where the emitting layer is a blend of a small molecule and a polymer.

There is a lack of investigation into the complexities of a mixed EML where the emissive species interact with each other, with little to no calculations that predict emission from multi-emitter devices. Recently, a simulation technique was developed [24], which allows for fast optimization of OLED geometries, addressing design problems. This technique is based on the scattering matrix method that has been very successful in simulating the optical properties of photonic crystals [25,26]. It can be applied to OLEDs [27] and is applied here to understand the mechanisms underlying the mixed emitting layer devices.

A blend of PVK and CBP was used previously, at various ratios, as a host for Ir-complex emitters requiring a high gap host [28-30]. In these previous studies, PVK was the matrix, while CBP was the charge carrier transport material. In this work, the PVK:CBP blend is used as a mixed emitter to enable realization of UV and deep-blue μ c emissions for use in a compact tunable solid-state UV source, such as an OLED-based on-chip spectrometer. The combination

of PVK and CBP expands the blue-region emission compared to a CBP-only device, enabling μ c devices to extend to $\lambda \sim 469$ nm, compared to $\lambda \sim 428$ nm in the CBP only device [31].

Using the combined emission of PVK and CBP as a base for μ cOLEDs, we are able to produce multiple emission peaks by varying the thickness of the hole injection layer MoO_x and electron transport layer 4,7-diphenyl-1,10-phenanthroline (BPhen). In an effort to understand and improve the emission properties of such μ c devices, the origins of the source emission are investigated using scattering matrix-based simulations. The simulations suggest that the spontaneous emission rates strongly depend on the local electric fields at the emitting sites. Consequently, the contributions from PVK and CBP EL to the total spectrum are dependent on the optical cavity length.

2. Experimental

OLEDs were fabricated on nominally 12 Ohm/sq, 140 nm-thick ITO-coated glass substrates or on the same glass substrates with ITO removed. The substrates were cleaned as detailed in the Supplementary Information (SI) section. They were treated with UV-ozone to increase the work function of ITO. On the plain glass substrates, 40 nm silver was deposited by thermal evaporation. MoO_x was then deposited on all substrates using a sliding shutter to control thicknesses. The EML solution, a mixture of PVK and CBP with total concentration of 9 mg/mL in chlorobenzene, was spin-coated in a nitrogen-filled glovebox (< 20 ppm O_2) atop the MoO_x , then baked at 60°C for 30 min and pumped in the thermal evaporation system overnight to remove residual solvent. Atomic force microscopy (AFM) scans were used to obtain the root-mean-square roughness (R_{RMS}) and the related spread for the films. Devices were fabricated by

evaporating subsequent layers, including 4,7-diphenyl-1,10-phenanthroline (BPhen) (an electron transport/ hole blocking layer), LiF cathode buffer, and Al. The structure was:

ITO or 40 nm Ag/5,10,15, or 20 nm MoO_x/~30 nm PVK:CBP/10,15,20, or 30 nm BPhen/1 nm LiF/100 nm Al. The resulting devices were 1.5 mm diameter disk-shaped pixels.

Devices were characterized by current density-voltage measurements and by EL spectra.

Additional fabrication information is presented in the SI.

3. Theory and Calculation

In the scattering matrix formalism the OLED is composed of layers stacked in the z direction. In each layer of the OLED stack, the materials are represented by realistic frequency dependent absorptive dielectric functions obtained from experimental measurements of N,N'-bis-(3-naphthyl)-N,N'-biphenyl-(1,1'-biphenyl)-4,4'-diamine (NPB) [32], Ag [33], MoO_x [34] and ITO [33]. Rather than assuming that all layers are planar in the (x,y) plane we have adopted a more general formalism where the layers can have a periodic structure in the planar (x,y) directions with a repeat vector $\mathbf{R} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2$, where the primitive lattice vectors are $\mathbf{a}_1$ and $\mathbf{a}_2$. This general formalism allows for the investigation of outcoupling of trapped modes using periodic microlens structures or grating structures.

Within each layer of the OLED structure the dielectric function $\epsilon(x,y)$ is a function of x and y but not z , so its Fourier expansion is

$$\epsilon(r) = \sum_G \epsilon(G) e^{i\mathbf{G} \cdot \mathbf{r}} \quad (1)$$

where $\mathbf{G}$ are the reciprocal lattice vectors of the system. The electric and magnetic fields are also expanded in Fourier components with strengths given by

$$E_\alpha(r) = \sum_{i=1}^{N_G} e_{Gi,\alpha}(z) \exp(-i(k + G_i) \cdot x_\parallel) \quad (2)$$

The emissive source is described through the well-developed scattering matrix formalisms [25,26] as an infinitesimal dipole at position (r_0, z_0) within the emissive zone of the OLED, and described by an emissive dipole with strength J , which is also expanded in a Fourier series:

$$J(r, z) = J_0 \delta(r - r_0) \delta(z - z_0) = \sum_{k, G} j_k(G) \exp(i(k + G) \circ r) \delta(z - z_0) \quad (3)$$

where $j_k(G) = J_0 \exp(-i(k + G) \circ r_0)$.

The emission intensity is directly proportional to the strength of the source term J_0 . The amplitude of the dipole source J_0 depends on the rate of spontaneous emission, which in turn depends on the photon density of states (DOS) at the location of the dipole. The emission rate can be substantially modified from the free-space value due to cavity effects.

Following classical electromagnetism, the amplitude of the dipole source J is a *current* that is a radiative source term for Maxwell's equations. This current is distinct from the electron and hole currents in the OLED. With the OLED source term, Maxwell's equations for each frequency ω are:

$$\nabla \times H = J - i\omega \epsilon(r) E \quad (4)$$

$$\nabla \times E = i\omega H \quad (5)$$

Maxwell's equations in Fourier space can be compactly represented as:

$$i \hat{k}_y h_z(z) - h_y'(z) = j_x \delta(z - z_0) - i \hat{\epsilon} e_x(z) \quad (6)$$

$$h_x'(z) - i \hat{k}_x h_z(z) = j_y \delta(z - z_0) - i \hat{\epsilon} e_y(z) \quad (7)$$

$$i \hat{k}_y h_z(z) - i k_y h_x(z) = j_z \delta(z - z_0) - i \hat{\epsilon} e_z(z) \quad (8)$$

where e and h represent the Fourier component of the electric and magnetic fields, respectively, in matrix form. $\hat{\epsilon}$ is the Fourier transformed dielectric function in matrix form and $\hat{k}_y$ is the diagonal matrix $(k+G)_x$.

At all layers of the OLED other than the emissive layer the parallel components of the electric and magnetic fields (E_x, E_y) and (H_x, H_y) are continuous. However, in the layer containing the emissive source the parallel components of the electric and magnetic fields are discontinuous. For an emissive dipole oriented in a random direction between layers l and $l+1$, the discontinuity of the fields is [25]

$$\begin{aligned} e_{\parallel}^{l+1}(0) - e_{\parallel}^{l+1}(d_l) &= p_z \\ h_{\parallel}^{l+1}(0) - h_{\parallel}^{l+1}(d_l) &= p_{\parallel} \end{aligned} \quad (9)$$

where p_z and $p_{\parallel}$ are the normal and in-plane components, respectively, of the dipole moments in the emissive layer [25].

The remaining layers can be treated with the standard scattering matrix formalism used in photonic crystals [35]. Within each layer the fields satisfy transfer matrix equations relating the Fourier components of the E fields to the H fields and vice-versa.

$$\frac{\partial}{\partial z} E = M_1 H; \frac{\partial}{\partial z} H = M_2 H \quad (10)$$

$$\frac{\partial^2}{\partial z^2} E = M_1 M_2 E \quad (11)$$

Here M_1 and M_2 are transfer matrices with dimension $(2N_G \times 2N_G)$, where N_G is the number of Fourier components. Both polarizations are automatically simulated and the eigenvalue equation (Eq. 11) is solved to obtain the normal modes within each layer. Individual scattering matrices (s_i) are computed with each layer. A standard convolution algorithm [35] links the scattering

matrix of the emissive layer to that of the air region above the OLED, from which the emission is obtained.

The simulation of the emitted fields is obtained for each three-dimensional orientation of the dipole, which is summed to obtain the total emitted field in the air region. This approach was very successful in simulating the wavelength dependent emission and the penetration of fields within the metals in μ OLEDs, when the MoO_x spacer layer thickness was varied [16].

4. Results and Discussion

4.1. ITO-based devices and source profile

A mixed emitting layer (EML) composed of PVK and CBP that results in a broad EL band (when ITO is the anode) can be used for generating UV-to-blue μ c pixel arrays. Different PVK:CBP weight ratios, including 1:1, 2:1, and 3:1, were tested first in ITO-based devices to optimize a wide emission spectrum, as shown in **Figure 1(a)**. The device structures were: ITO/5 nm MoO_x /EML/20 nm BPhen/1 nm LiF /100 nm Al. As expected, with increased PVK weight fraction, the longer wavelength emission, seen only in the PVK EL spectrum, is more prominent. Interestingly, a PVK:CBP ratio that results in a broader EL spectrum in ITO-based OLEDs yields narrower full widths at half maximum (FWHMs) μ c emission bands for devices optimized for longer wavelength peaks, such as for the device with the ~ 440 nm peak shown in **Figure 1(b)**. As can be seen, the μ c devices made from 3:1 PVK:CBP ratio have a narrower FWHM and a weaker shoulder at shorter wavelengths. The FWHM and spectral shape of the μ c bands at shorter wavelength, however, are not altered with increasing PVK fraction.

Figure 1. EL spectra of (a) ITO-based devices with EMLs of various PVK:CBP ratios and (b) microcavity devices with emission peak at ~440 nm using different EMLs.

To better understand the emission profiles of μc structures with the PVK:CBP 3:1 EML, analogous ITO-based devices (differing by only the anode) with different MoO_x thicknesses were tested. The structures were: ITO/5, 10, 15 or 20 nm MoO_x /~30 nm 3:1 PVK:CBP/20 nm

BPhen/1 nm LiF/100 nm Al. **Figure 2(a)** shows the emission spectra of these devices. Although for a given device structure there is a slight spectral shift with change in applied voltage (not shown), the variations between pixels are minimal. It is clear that with increasing MoO_x thickness, the emission is narrowed (FWHM decreases from 77 nm to 61 nm) and red-shifted (peaks shift from ~391 nm to ~406 nm). This is consistent with the known weak μc effect even in devices with a non-metallic anode [36]. **Figure 2(b)** shows the calculated curves, discussed below, which match well to the red-shift and narrowing of the measured spectra.

Figure 3(a) shows the current density vs. voltage $J(V)$ curves for ITO-based devices with MoO_x thickness of 5, 10, 15, or 20 nm and BPhen thickness of 20 nm. The typical variation of these $J(V)$ curves is approximately $\pm 10\%$. It is clear that at a given voltage, increasing the MoO_x thickness increases the current, with the largest difference being between 5 nm and 10 nm thick MoO_x devices. In previous studies, the current decreased with increasing MoO_x thickness, presumably due to the increase in resistance from the thicker MoO_x [16].

Atomic force microscopy (AFM) images of the MoO_x films were taken to determine the cause of the contrasting characteristic seen here. **Figure S1** shows the AFM images of ITO/MoO_x films with MoO_x thicknesses of 5 and 20 nm; the root-mean-square roughness (R_{RMS}) values are shown in **Table S1** for MoO_x thicknesses of 5, 10, 15, and 20 nm. Images corresponding to the additional RMS values in **Table S1** are discussed later.

Figure 2. Spectra of ITO-based 3:1 PVK:CBP devices with various MoO_x thicknesses (20 nm BPhen), (a) measured and (b) calculated.

Figure 3. Current density vs. voltage of ITO-based devices with (a) various MoO_x thicknesses (20 nm BPhen) and (b) various BPhen thicknesses (15 nm MoO_x).

The roughness of MoO_x does not change significantly with changing thickness and mirrors the underlying ITO layer roughness, known to be ~ 4.4 nm [37]. It is therefore likely that the 5 nm MoO_x on ITO is significantly discontinuous, having a roughness similar to its thickness. The thin, discontinuous layer would have poorer injection and, consequently, lower current compared to the thicker, more continuous MoO_x layers.

Current density vs. voltage for ITO-based devices with changing BPhen thickness (10, 15, 20, and 30 nm), but constant MoO_x thickness (15 nm), are shown in **Figure 3(b)**. The current decreases slightly at a given voltage with increasing BPhen thickness, likely due to increased resistance from the thicker BPhen.

In order to predict the μ c emission with the PVK:CBP EML, the source profile is determined by comparing simulations with measurements for the ITO-based device with 5 nm thick MoO_x and 20 nm thick BPhen (variations of the source profile with thicker MoO_x were small). The emitting species is represented by infinitesimal dipoles residing within the PVK:CBP blend layer. The transmission intensity $T_{cal}(\lambda)$ from the ITO-based device in all directions is simulated using these emissive sources (via the scattering matrix method). The source profile $I_{source}(\lambda)$ of the emitting source is then fitted to the measured data through the relation:

$$E_{meas}(\lambda) = T_{cal}(\lambda) \cdot I_{source}(\lambda) \quad (12)$$

where $E_{meas}(\lambda)$ is the experimentally measured emission (in the normal direction). The extracted source profile is shown in **Figure 4(a)**, after smoothing of the simulated data.

To reduce multiple interference effects, the simulations are averaged over a 0-10° angle of emission. The source profile has i) a sharp peak near 370 nm and ii) a broad tail at longer wavelengths extending beyond 550 nm, which may then be conveniently decomposed into two Gaussians. The Gaussian centered at ~370 nm represents emission from CBP, with the peak at

~420 nm representing emission from the PVK (**Figure 4(a)**). Because the sum of the two Gaussians matches closely the experimentally derived source profile, there is little evidence for secondary emission such as that from excimers. The two Gaussians are similar to the experimental EL spectra for neat CBP and neat PVK (shown in **Figure 4(b)**), strengthening the model analysis.

Figure 4. EL spectra of (a) the source profile calculated from the experimental data and extracted Gaussian fits and (b) neat CBP and PVK.

The source profile is used to simulate the emission from ITO-based devices as a function of the MoO_x thickness (**Figure 2(b)**). The red shift and narrowing of the emission spectrum with increasing MoO_x thickness predicted by simulations agrees well with that measured.

4.2. Microcavity devices

Figure 5(a) shows the EL spectra of μc devices of the structure: 40 nm Ag / x nm MoO_x / ~30 nm 3:1 PVK:CBP / y nm BPhen / 1 nm LiF / 100 nm Al, where $x = 5, 10, 15$, or 20 nm and $y = 10, 15, 20$, or 30 nm. To optimize the μc EL peaks, the thickness of MoO_x and BPhen were changed. It was shown previously that thicker Ag gives narrower peaks, at the expense of transparency and so 40 nm silver is used here instead of the more efficient 25 nm thickness [16]. The emission peaks can be tuned from 373 to 469 nm, with FWHM ranging from 21 to 41 nm (see **Table 1**). At longer wavelengths, the FWHM is wider, likely due to the lower intensity of the source profile at these wavelengths.

Figure 5. *EL spectra of μ COLEDs: (a) measured and (b) calculated.*

Table 1. Layer thicknesses and measured and best-fit calculated spectral characteristics

Measured Spectra				Best-Fit Calculated Spectra			
MoO _x (nm)	BPhen (nm)	Peak λ (nm)	FWHM (nm)	MoO _x (nm)	BPhen (nm)	Peak λ (nm)	FWHM (ave. 0-10°) (nm)
5	10	373	21	2	7	378	46
5	20	391	28	4	15	392	46
10	15	403	34	10	15	400	37
5	30	410	34	5	30	414	23
15	10	420	41	23	15	421	33
15	15	429	41	22	22	428	29
15	20	441	47	20	30	442	36
20	10	452	50	32	20	450	47
15	30	469	41	20	40	471	49

Figure 6 shows the J - V curves of μc devices of the structure: 40 nm Ag/5,10, or 15 nm MoO_x/3:1 PVK:CBP/20 nm BPhen/1 nm LiF/100 nm Al. The μc devices show the same trend as the ITO-based devices, though not as pronounced, in that the current increases at a given voltage with increasing MoO_x thickness. The irradiance of the μc device with the 15 nm MoO_x was 0.45 mW/cm² at 1.6 mA/cm². This irradiance is larger than the 0.33 mW/cm² obtained for a μc device with a neat CBP EML [31]. **Figure S4** shows the current density and the irradiance vs voltage for this device.

Figure 6. *Current density vs. voltage of μc devices with various MoO_x thicknesses.*

Initial simulations, performed to fit the experimental μc peaks (see **Figure 5(b)**), used the source profile calculated from the ITO-based device with 5 nm MoO_x and 20 nm BPhen, shown above.

It can be seen that the initial fit is poor at the shortest wavelengths, best in the mid-range, and fairly good at the long wavelengths. The thicknesses used in the simulations differ slightly from the experimental values in order to match the peak wavelength, as listed in **Table 1**. It is possible that the experimental thicknesses are not precise, as the spin-coated layer thickness was estimated from AFM measurements, and the thickness monitor, which measures the evaporated layers, is subject to systematic errors resulting from inaccurate parameters, such as the acoustic impedance and material density, as well as variations in the positions of the sample and the quartz probe of the thickness monitor in the evaporation chamber.

Since the short wavelength fits were unsatisfactory, we next used a different approach to simulate the spectra. In this approach, each Gaussian source profile is multiplied by the calculated transmission profile $T_{cal}(\lambda)$ of the shortest optical length device ($t_{MoO_x} = 2$ nm, $t_{BPhen} = 7$ nm). Similarly, the two Gaussian profiles were also multiplied by the calculated transmission profiles for the longest optical length device ($t_{MoO_x} = 20$ nm, $t_{BPhen} = 40$ nm), see **Figure 5**. The results are shown in **Figure 7**. The best fit suggests that at shorter wavelengths, the emission is almost entirely from CBP, while at longer wavelengths the emission from PVK is more prevalent, with a weak shoulder at short wavelengths due to CBP. The best-fit simulation for the μ c device emission therefore suggests differing source profiles for devices with different optical lengths.

The deviations of the simulated spectra from the observed profiles may be due to (i) the inaccurate values of the refractive index $n(\lambda)$ for MoO_x , which likely depend on x , and (ii) the unknown $n(\lambda)$ for CBP and PVK, which may differ significantly from $n(\lambda)$ of NPB that was used for all of the organic layers.

To determine the cause of the optical length-dependence of the source profiles, we also investigated the effects of MoO_x thickness on the morphology of the organic layers. AFM images of the Ag/ MoO_x films, with MoO_x thicknesses of 5, 10, 15, and 20 nm, and of the spin-coated EML on [ITO or Ag]/ MoO_x were taken. R_{RMS} values are listed in Table S1 and selected images are shown in **Figures S2 and S3**.

It can be seen that the MoO_x film on silver is much smoother than on ITO and it does not vary significantly with MoO_x thickness. The smooth MoO_x layers indicate that there is likely no dependence of the spin-coated layer morphology on device structure. AFM scans of the EML on [ITO or Ag 40 nm]/ MoO_x [5 or 20 nm] show that the PVK:CBP layer is smooth ($R_{RMS} \leq 1$ nm),

slightly more so with Ag than with ITO. Previous studies have shown that smooth AFM images correspond to films that are homogeneous [38-40]. We therefore conclude that the PVK:CBP is likely not phase separated or aggregated.

To roughly visualize the homogeneous mixture of PVK and CBP, the two can be approximated as spheres, as PVK's unconjugated backbone likely coils upon itself (see **Figure 8**) [40].

PVK has a molecular weight between 25,000 and 50,000, compared to the small molecule CBP whose molecular weight is ~485. Therefore PVK's spherical radius would be ~4–5 times that of CBP. The random binary mixture of spheres (with a volume ratio of the two components similar in the present work) simulated in a previous study by A. V. Kyrylyuk et al. [41] suggests a percolating network of the smaller CBP molecules surrounding the larger PVK molecules (see **Figure 8**), despite the 3:1 PVK to CBP weight ratio. This structure has implications for charge transport, as described in the next section.

Figure 7. Measured EL spectra and spectra calculated individually from the two Gaussian source profiles for (a) 373 nm and (b) 469 nm experimental peaks.

Figure 8. a) Molecular structure of PVK and CBP. b) Schematic representation of packing of CBP and PVK molecules. Not all CBP molecules are shown.

5. Role of the Photon Density of States (DOS)

The simulation presented above takes into account the optical properties of the materials, which include their wavelength-dependent real and imaginary components of the dielectric function and thicknesses. However, the simulations did not consider the effects of changes in the photon DOS, which result in changes in the emission rates depending on the cavity resonant frequency. The spontaneous emission rate R is dependent on the dipole transition matrix element and the DOS, as expressed by:

$$R = \frac{2\pi}{\hbar} |M_{ij}|^2 \rho(\omega) \quad (13)$$

M_{ij} is the dipole transition matrix element, $\rho(\omega)$ is the photon DOS, and ω is the frequency.

Therefore, if the DOS increases at the resonant frequency, R increases at that frequency. The current computational program does not incorporate this field enhancement factor into the intensity and requires the excitation current J_0 (Eq. 3) to be a function of λ that also depends on the local DOS, rather than a constant value.

Based on the foregoing multi-component structure [41] (**Figure 8(b)**) and the much higher electron and hole mobilities in CBP in comparison to PVK, almost all charge transport occurs in the percolating CBP matrix [42]. Moreover, within the PVK:CBP layer, the electron density in the PVK component is likely much lower than that in CBP as the PVK's LUMO level is 0.5 eV above that of CBP, see **Figure 9**. Therefore, it is likely that most excitons form on CBP.

However, as there is still obvious PVK emission in the long optical length devices, some excitons form on or transfer to the slightly lower gap sites on PVK molecules. We also suspect that as the HOMO level of PVK is shallower than that of CBP, it likely traps holes in coiled sites (see Figure 11(b)) [40]. We note that while the absorption edge of PVK is at shorter wavelength than that of CBP, the source emission of CBP is at shorter wavelength, i.e., the Stokes shift of

PVK is considerably larger than that of CBP. This is plausible given the likelihood that the PVK emission site is more disordered than that of CBP, and emission from PVK occurs from sites that, on average, are deeper exciton trapping sites than those from CBP.

In the thin cavity devices, the short wavelength R is increased, implying that CBP will likely emit faster, lowering the chance for charge or energy transfer to PVK. In thick cavity devices, the long wavelength R is increased, possibly increasing the likelihood of PVK emission occurring before the exciton can dissociate and transfer an electron into the CBP LUMO. A direction for future simulation would be to include the dependence of excitation rates on the wavelength and OLED geometry.

Figure 9. Energy diagram of the materials used in OLEDs.

6. Conclusions

A mixture of PVK and CBP at a ratio of 3:1 was used to create a broad-band source profile, optimized for use as the EML in tunable microcavity OLEDs. Narrow deep blue-UV emissions

(FWHM $\sim 20 - 40$ nm) in the range of $\lambda \sim 373 - 469$ nm were obtained from 2-d combinatorial arrays of such devices. The source profile was extracted from an ITO-based device emission spectrum and used to calculate the microcavity EL spectra. It was found that the calculated spectra represented well the experimental spectra at longer wavelengths (> 400 nm), but did not match well at short wavelengths, likely because the simulation did not take into account the effect of the change in the photon density of states and the resulting wavelength-dependent emission rate in the short wavelength regime. The work highlights interesting characteristics of the emission of a mixed EML, the effects of the component attributes, and the resultant difficulties in simulating the emission. Potential refinement of the simulations includes the analysis of real space electric fields and better understanding of the electron and hole transport within the mixed emitters. The UV and deep-blue narrow band multicolor OLED pixels should be usable for an expanded wavelength range of on-chip spectrometers as well as for other analytical applications.

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Deep blue/ultraviolet microcavity OLEDs based on solution-processed PVK:CBP blends

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Keywords

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