Supporting Information

Defect Engineering in Organic Semiconductor Based Metal-Dielectric Photonic Crystals

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1 Photonic Bandwidth Narrowing

The normal emission profiles from both simulated (shown in main Figure 2) and experimental results for the $N = 3$ MDPC device with $t_{\mathrm{org}} = t_{\mathrm{s}} = 350$ nm and total thickness of approximately 1050 nm, as illustrated in Figure **1**, demonstrate a photonic band structure that preserves the central peaks of each band, similar to those observed in the $N = 1$ device. The vertical dotted red and blue lines at wavelengths $\lambda_2 = 691$ nm and $\lambda_3 = 483$ nm, along with the vertical dashed red and blue lines at $\lambda'_2 = 698$ nm and $\lambda'_3 = 486$, mark the centers of the photonic bands for the $j = 2$ and $j = 3$ modes, respectively, as observed in the simulations (λ_j) and experiments (λ'_j). The full widths at half maximum (FWHM) of the central peaks of teh $j = 2$ and $j = 3$ bands are approximately 9.3 nm and 6.9 nm for the simulated spectrum, as determined by multi-peak fitting. The linewidths of the same peaks in the experimental spectrum are 8 nm and 6.5 nm. The simulation results indicate that the bandwidths for the $j = 2$ and $j = 3$ bands are 85 nm and 43 nm, respectively, while the experimental results show bandwidths of 64 nm and 37 nm.

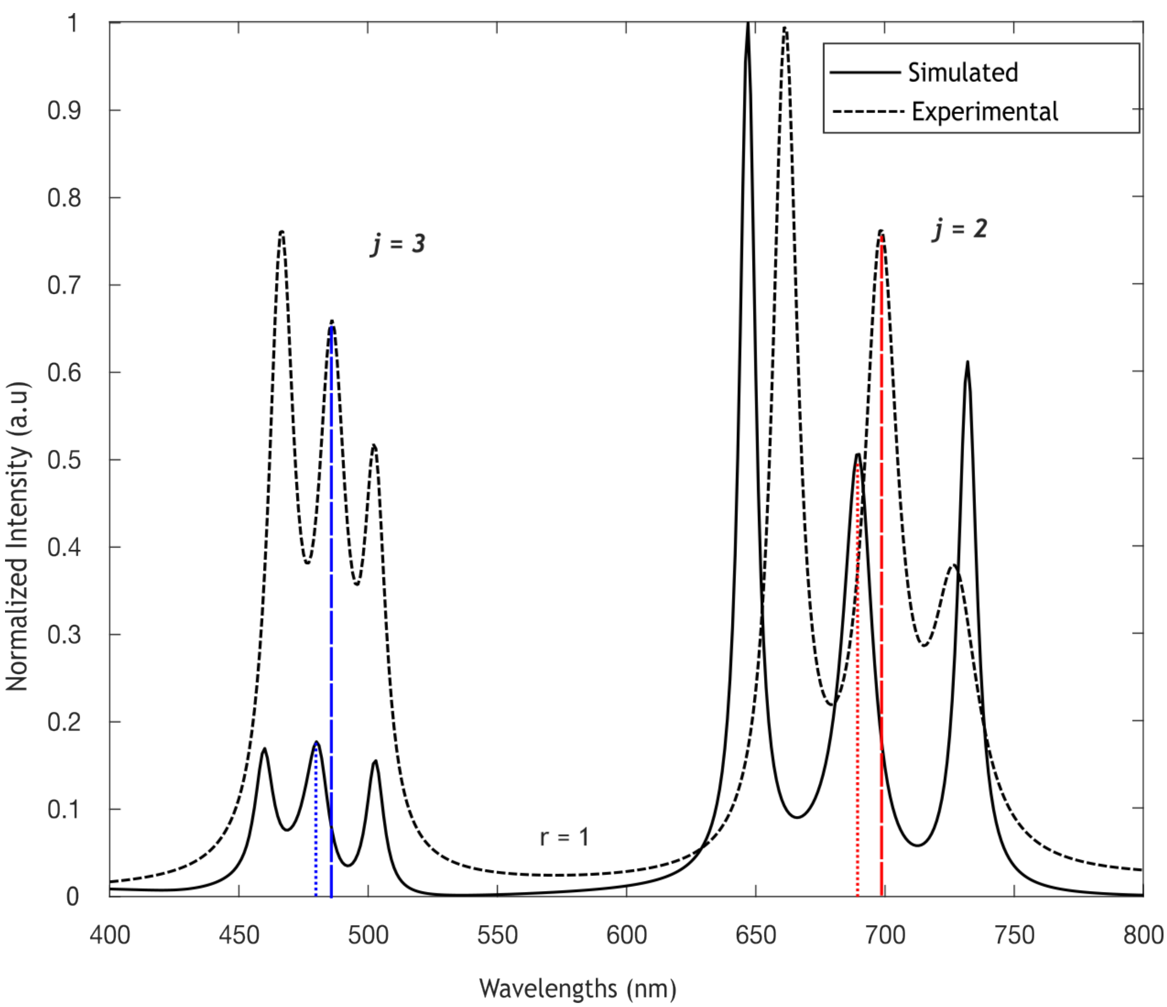

Figure 1: Comparision of simulated and experimentally observed photonic bands from the $N = 3$ MDPC device, with $t_{\mathrm{org}} = t_{\mathrm{s}}$ and the standard cavity of size 300 nm.

2 Behaviour of a Larger MDPC (for $N = 5$)

We investigate the behavior of multilayer dielectric photonic crystals (MDPCs) with more complex configurations by introducing a defect into an $N = 5$ cavity MDPC structure. The results, illustrated in Figure **2**, reveal a behavior analogous to that observed in the simpler $N = 3$ cavity case. These findings suggest that the observed phenomena can be extended to larger MDPC crystals. Figure 2 shows the emission patterns from $N = 5$ MDPC structure for a full range of defects from $0.02 \leq r \leq 2.0$ for a center cavity defect **(a)**, an intermediate cavity defect **(b)**, and an edge cavity defect **(c)**.
Deviating either side from $r = 1$ results the lowest energy state migrating from each band into the band gap, resulting in four states remaining in the band. These four remaining states in the band converge either closely and become nearly degenerate or stay as distinct states in the band depending on the position of the defects in the crystal. If the defect were situated in the central cavity shown in Figure **(a)**, the extreme scenario of the defect would uncouple the two leftmost and the rightmost static cavities from the central cavity and from each other. This results the two lowest energy states and two higher energy states collapse onto each other, nearly reaching degeneracy, identical to the $N = 2$, uncoupled microcavity system. Conversely, when the defect occurs in an edge cavity as shown in Figure **(c)**, it displays the characteristic behavior of an isolated defect state and $N = 4$ coupled resonator system, featuring four distinct states within the band. In the context of the intermediate cavity defect shown in Figure **(b)**, the three static cavities—either the leftmost or rightmost static cavities relative to the intermediate cavity, and the edge cavity—would be isolated from both the intermediate cavity and each other. This results the mixture of degenerate and non-degenerate energy states identical to the $N = 3$ and $N = 1$ uncoupled microcavity system.

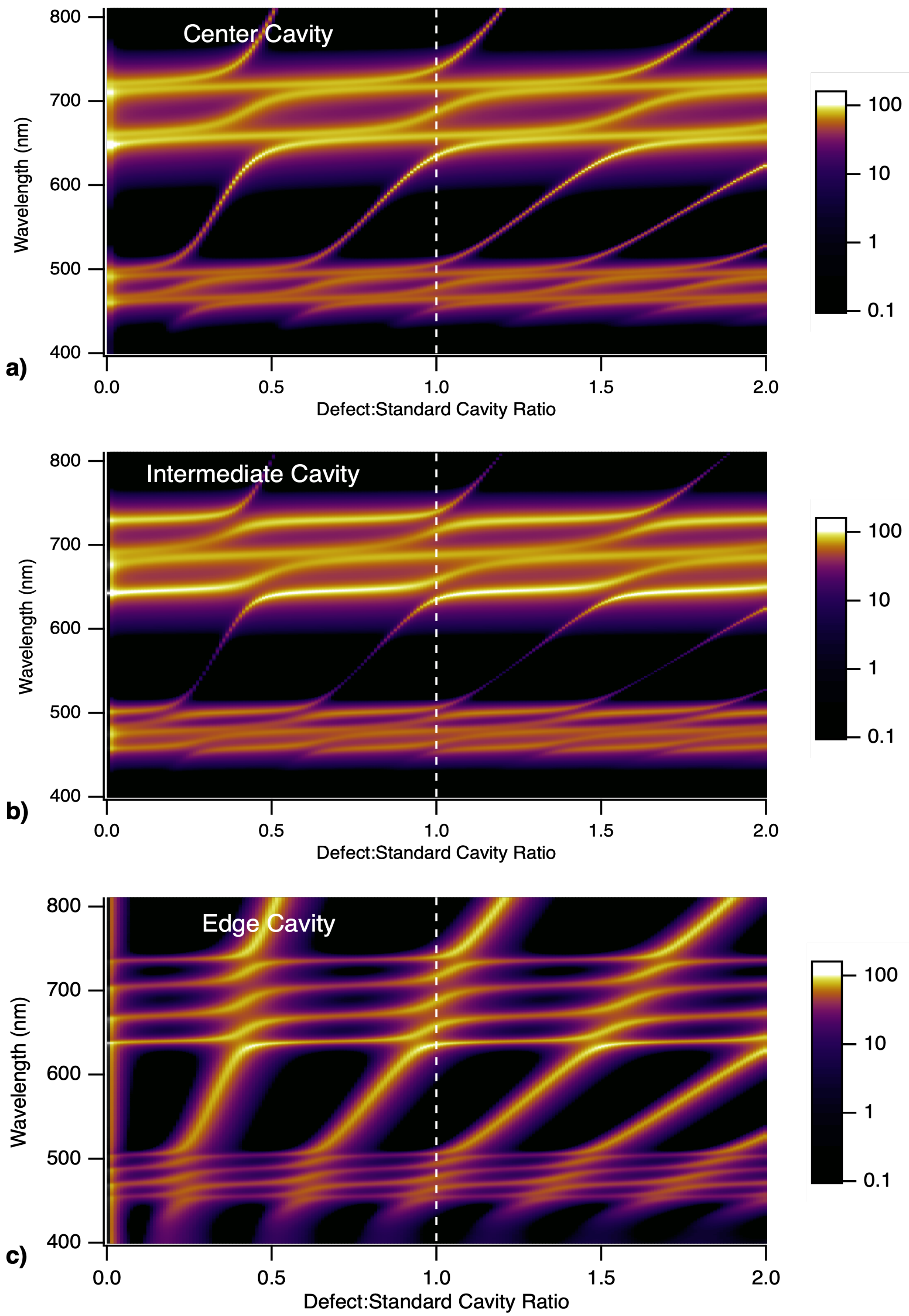

Figure 2: A normal emissions from a $N = 5$ cavity MDPC device for a full range of defects from full $0.02 \leq r \leq 2.0$ with **(a)** defect in the center cavity, **(b)** defect in the intermediate cavity (cavity between center and edge), and **(c)** defect in the edge cavity. The central white lines in all three figures represent the absence of defects, indicated by $r = 1$. "Resonant" crystal states manifest at anti-crossings.

3 Perturbation and Energy Bands

For a $N = 1$ (single cavity), the general resonance condition with the consideration of the penetration depth in mirrors can be expressed as [2]

$$\lambda_j = \frac{2}{\left[j - 2\left|\frac{\phi^{\uparrow}+\phi^{\downarrow}}{4\pi}\right|\right]}\sum_i n_i t_i \qquad j = 1, 2, 3, \ldots \tag{1}$$

Where, $\phi^{\uparrow}$ and $\phi^{\downarrow}$ are the phase shifts at the top and bottom mirrors, n_i and t_i represent the index of refraction and thickness of each active layers between mirrors, $\sum_i n_i t_i$ is the optical path length, λ is the wavelength of the state, and j is any natural number. With the introduction of our mirrors, dividing our device into a crystal, the electric field will be perturbed. The perturbation affects the wavelength of the states, and causes the formation of energy bands, as described by Allemeier et al. [1]. When we look at a $N = 3$ non-defect device ($r = 1$) with the standard cavity of thickness 100 nm, we see electric field profiles of the three states that constitute the $j = 1$ band in Figure **3**.

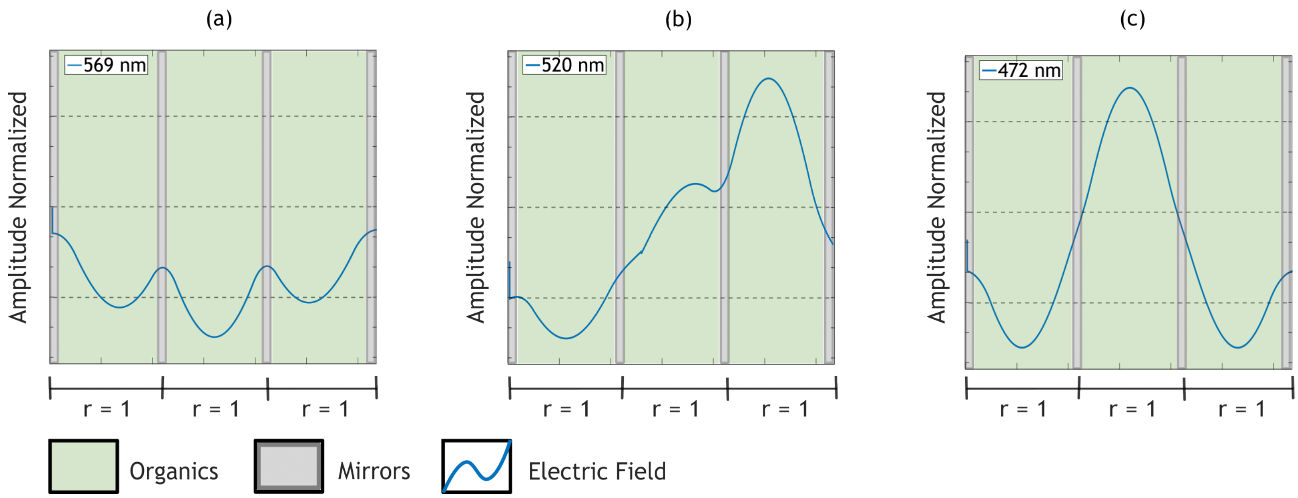

Figure 3: Resonant states $\lambda/2$, λ, and $3\lambda/2$ of the fundamental band from a $N = 3$ MDPC device with the standard (static) cavity of size 100 nm.

In these figures, we can see that the $3\lambda/2$ state is hardly perturbed at all, while the $\lambda/2$ state has had the most perturbation given that the mirrors (which act loosely as nodes) are near the anti-node of the state. Greatly perturbed states have their energies shifted upwards significantly. This is the phenomenon that results in band formation of the energy states. As we begin to defect the cavity, the perturbation of each state will change.
In the case of +26% ($r = 1.26$) defect in the center cavity shown in Figure **4**, the levels of perturbation have changed. The $\lambda/2$ state has seen a decrease in perturbation as the mirrors move outwards, away from the center anti-node. This, combined with the increase in the optical path length, has resulted in a drastic increase in peak wavelength. The λ state is seeing an increase in perturbation as the mirrors move outwards towards its anti-nodes. The increase in perturbation causes a decrease in the peak wavelength that is at odds with the increase in peak wavelength expected from the increase in optical path length. The state has been perturbed to the point where it is almost completely unrecognizable. The $3\lambda/2$ state has seen an increase in perturbation, as it was previously at a perturbation minimum. This perturbation prevents the state from changing too drastically in wavelength from the shift in

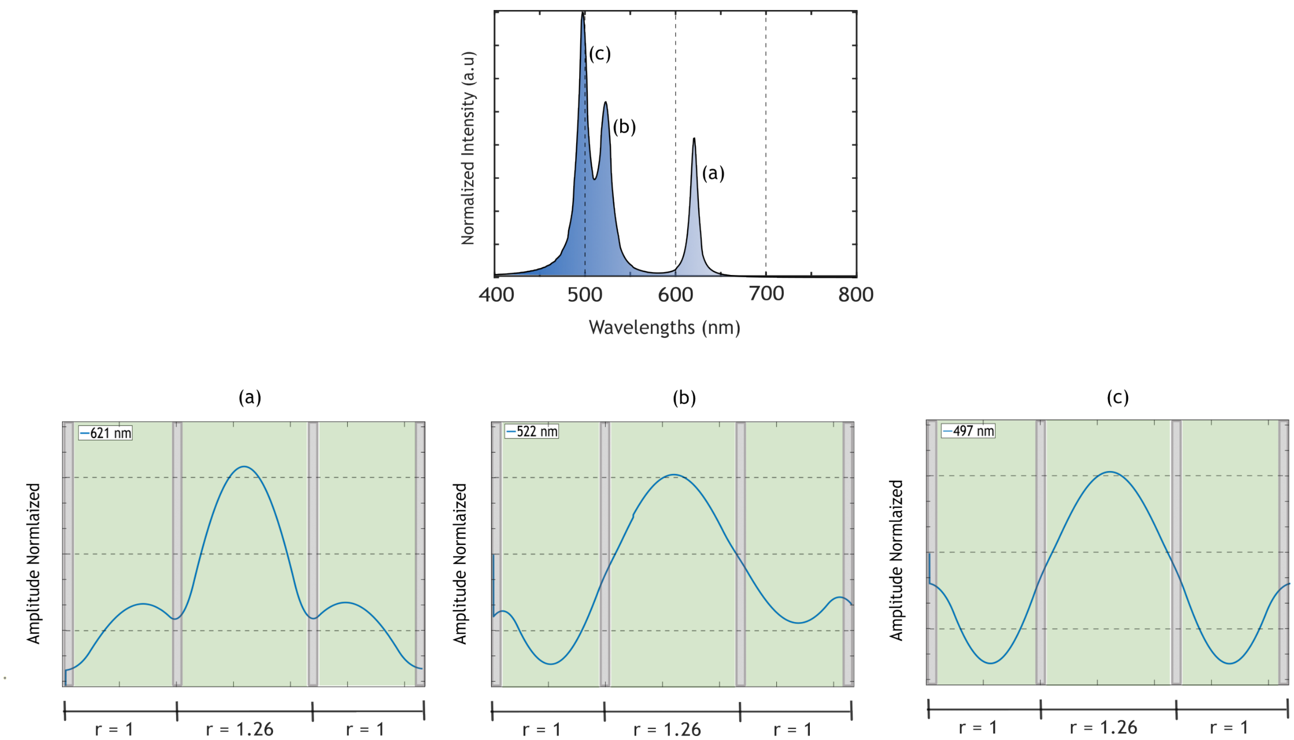

Figure 4: Showing normalized intensity (top row) and corresponding energy states (bottom row) $\lambda/2$, λ, and $3\lambda/2$ of a $N = 3$ MDPC device with the defect $r = 1.26$ in the center cavity.

cavity size. This pattern continues for some time, with the mirrors moving outwards, and the levels of perturbation changing until the system eventually reaches a resonance condition.

References

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