UniMCO 4.0: A Unique CAD Tool for LED, OLED, RCLED, VCSEL, & Optical Coatings
Outline

• Physics of LED & OLED
• Microcavity LED (RCLED) and OLED (MCOLED)
• UniMCO 4.0: Unique CAD tool for LED-Based Devices
  – Key Features
  – Extensive Material Database
  – Automatic EL0 Extraction from Experimental Data
  – Built-in Device Structure Library
  – Device Optimization
  – Optical Function Calculations
  – Comprehensive 2D and 3D Post-Processor
• Case Studies Using UniMCO 4.0
• Why UniMCO?
Physics of LED & OLED

- Device Structures (Multi-layers):

A Typical OLED Structure

A Typical RCLED (or VCSEL) Structure
Physics of LED & OLED

• External quantum efficiency of LED & OLED:

\[ \eta_{\text{ext}} = \eta_{\text{inj}} \eta_{\text{rad}} \eta_{\text{extr}} \]

• \( \eta_{\text{inj}} \): Fraction of carriers injected in active region (charge balance between anode & cathode).

• \( \eta_{\text{rad}} \): Radiative fraction of spontaneous recombination (singlet-triplet ratio, impurities, …)

• \( \eta_{\text{extr}} \): Extraction efficiency of generated photons (complete internal reflection, emitting zone location, microcavity effect, …)
Physics of LED & OLED

- Electrons to photons conversion in LED & OLED (display application)

![Diagram showing the process of electrons to photons conversion in LED & OLED](image)

- Injected carriers
- Carriers in active region
- Generated photons
- Extracted photons
- Photons in outside

\[ \eta_{\text{extr}} \]

- \( \eta_{\text{inj}} \) injected carriers
- \( \eta_{\text{rad}} \) non-radiative recombination
- \( \eta_{\text{extr}} \) extracted photons

Light coupled to wide view angle

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Physics of LED & OLED

- Electrons to photons conversion in LED coupled to waveguide or fiber (communication applications)

Injected carriers -> Carriers in active region -> Generated photons -> Extracted photons

- Photons in waveguide
- Not coupled to a small N.A.
- Only coupled to a small N.A.

- Injected carriers
- Carriers in active region
- Generated photons
- Extracted photons

- Not injected in active region
- Non-radiative recombination
- Not extracted
- Not coupled in waveguide

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Physics of LED & OLED

- **Charge Injection Efficiency** $\eta_{\text{inj}}$
  - OLED: improve anode & cathode materials to enhance charge balance (limited room to improve)
  - Semiconductor LED: $\sim 100\%$ (very little room to improve)

- **Light Radiation Efficiency** $\eta_{\text{rad}}$
  - OLED: doping leads to triplets to radiate light, … (limited room to improve)
  - Semiconductor LED: $\sim 70\% - 99\%$ (little room to improve)

- **Light Extraction Efficiency** $\eta_{\text{extr}}$
  - OLED: $< 20\%$ for most OLED structures (more room to improve)
  - Semiconductor LED $< 10\%$ in most case because of the large refractive index of the active layer (more room to improve)

- **Light Coupling Efficiency** $\eta_{\text{coupl}}$
  - RCLED: $\sim$ fraction of $\eta_{\text{extr}}$, coupled to optical fiber (more room to improve)

Extraction efficiency is the most important factor. The devices, if carefully designed, can increase $\eta_{\text{extr}}$ greatly.

UniMCO 4.0 can optimize the OLED & LED devices to enhance $\eta_{\text{extr}}$ & $\eta_{\text{coupl}}$. 

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• Microcavity can change spontaneous emission (SE):
  - Purcell Effect: Total Emission Enhancement

\[ r = +1: \text{perfect DBR mirror} \]
\[ r = -1: \text{perfect metallic mirror} \]
RCLED & MCOLED

Microcavity can improve extraction efficiency:

- **Bare in medium**: \( \eta \sim \frac{1}{4n^2} \)
  - \( n = 1.7 \): \( 8\% \)
  - \( n = 3.55 \): \( 2\% \)

- **Far from mirror**: \( \eta \sim \frac{1}{(2n^2)} \)
  - \( n = 1.7 \): \( 16\% \)
  - \( n = 3.55 \): \( 4\% \)

- **Close to mirror**: \( \eta \sim \frac{1}{n^2} \)
  - \( n = 1.7 \): \( 32\% \)
  - \( n = 3.55 \): \( 8\% \)

- **In big cavity**: \( \eta \sim \frac{1}{(2n^2)} \)
  - \( n = 1.7 \): \( 16\% \)
  - \( n = 3.55 \): \( 4\% \)

- **In small cavity**: \( \eta \sim \frac{1}{m_c} \)

Low order (small) microcavity is a key! \( L \sim \lambda \)
Difficult to get low order for DBR cavity:

Penetration depth (~ λ): Optical field penetrates into DBR layers, increasing the effective cavity length
Approaches to reduce the penetration depth:

- **Metal-DBR Microcavity** (almost no penetration to the metallic mirror)

- **Metal-Metal Microcavity** (almost no penetration to both metallic mirrors)
UniMCO 4.0: Key Features

- Advanced and easy to use CAD tool
- Extensive built-in material database for over 250 materials,
- Built-in library, including DBR-DBR cavity, Metal-DBR cavity, DBR-RCR cavity, Metal-RCR cavity, etc.
- Easy to build customized device structures using the built-in structure blocks, including substrate, DBR, spacer, emitter, and metal.
- Automatic light input (EL0) extraction from experimental data of a test structure
- Device layer thickness optimization by calculating optical field distribution.
UniMCO 4.0: Key Features

• Optimization of emitting zone location by calculating extracted EL spectrum
• Optical field distribution over whole device
• Optical functions as a function of various variables, including wavelength, view angle, and layer thickness.
• EL spectra for extracted, leaky, and guided modes
• Integrated EL and efficiency for extracted, leaky, and guided modes
• EL contributed from various polarization components: S-wave, P-wave, and vertical-wave.
• CIE XYZ 1931 and CIE LUV 1976 color coordinates for visible light and the color variation with view angle.
• Comprehensive 2D and 3D post-processors.
UniMCO 4.0: Material Database

- New feature of UniMCO 4.0
- Optical properties for over 250 materials
- Most commonly used materials in LED, RCLED, OLED, VCSEL, and optical coatings
- Intricate models that incorporate the effects of temperature and composition variations.
- Allows users to import material data through table or ASCII data
UniMCO 4.0: EL0 Extraction

- The accurate EL simulation depends on how good the input EL0 is.
- UniMCO requires the bare EL0 as input light spectrum.
- Even the experimental EL0 data from a specially designed test structure is still affected by the weak microcavity effect due to interfaces.
- EL0 extraction module can automatically remove the weak microcavity effect.
- The figure shows the extracted EL0 (red curve) from the experimental data (blue curve) of a test structure as illustrated in the top of the figure.
UniMCO 4.0: Built-In Structures

- UniMCO 4.0 has a built-in device structure library:
  - DBR-DBR structure
  - DBR-RCR structure (or double cavity structure)
  - Metal-DBR structure
  - Metal-non-DBR structure
  - Metal-RCR (double-cavity) structure

- From these 5 basic structures, we can build over 20 deduced structure by removing corresponding spacer layers.
UniMCO 4.0: Device Optimization

- **Layer Thickness Optimization**
  - Thickness variation affects EL output
  - Thickness variation results in color shift

The emitting layer thickness optimization for a GaAs/AlAs RCLED device at wavelength \( \lambda = 1300 \text{ nm} \) and view angle = 10 degree. The optimized thickness is \( 383.9 \text{ nm} \).
UniMCO 4.0: Device Optimization

- Emitting Zone Location Optimization
  - Emitting zone location affects EL output
  - To enhance EL, emitting zone must be at the anti-node of optical field
  - UniMCO 4.0 optimization module can predict the right emitting zone location

Emitting zone location optimization for a GaAs/AlAs RCLED device at wavelength = 1300 nm and view angle = 10 degree. The optimized emitting zone is at 205.6 nm.
UniMCO 4.0: Device Optimization

- **Example: OLED Optimization:**
  - Construct a device structure
  - Optimize ITO layer thickness and emitting zone location
  - Construct a microcavity OLED using optimized non-cavity device
  - Optimize HTL layer thickness and emitting zone
Optical function calculations

Optical Field Distribution:
- Optical field distribution provides the detailed information about the device structure

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Optical function calculations

- Reflectivity
- Transmittance
- Absorption
- Phase shift
Optical function calculations

Light Output:
- EL for extraction, leaky, guided modes
- EL for various polarized dipole models: s-wave, p-wave, & vertical
- Integrated EL over wavelength or view angle
- EL efficiency for extraction, leaky, guided modes
- Color coordinates for visible EL

A Unique CAD Tool for LED, OLED, RCLED, VCSEL, & Optical Coatings
Comprehensive 2D and 3D Post-Processor

Post-Processor Main Window (can display simulation results)

- Optical field ($\lambda$, x) or ($\Theta$, x)
- Reflectivity ($\lambda$, $\theta$), or ($\lambda$, d) or ($\theta$, d)
- Transmittance ($\lambda$, $\theta$), or ($\lambda$, d) or ($\theta$, d)
- Absorption ($\lambda$, $\theta$), or ($\lambda$, d) or ($\theta$, d)
- Phase Shift ($\lambda$, $\theta$), or ($\lambda$, d) or ($\theta$, d)
- EL ($\lambda$, $\theta$), or ($\lambda$, d) or ($\theta$, d)
2D Plots:
- 2D x-y plot
- Polar plot
- Linear or log scale
- Display multiple results on one plot
Comprehensive 2D and 3D Post-Processor

- 3D Plots
  - Surface plot
  - Contour plot
  - Linear or log scale
  - Color map control
Case Study 1: Multi-Wavelength Microcavity OLED

- Develop multi-wavelength white microcavity OLED device
- Enhance EL output
- Modify EL color

Material Parameters:
All material parameters are included in UniMCO’s material database except for CuPc. We use refractive index data for CuPc from literature: \( n = 1.5 - 0.8 \ i \).
Case Studies Using UniMCO 4.0

- Case Study 1: Multi-Wavelength Microcavity OLED

**CIE Color Coordinates:**

<table>
<thead>
<tr>
<th></th>
<th>Ref2</th>
<th>Cavity</th>
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<tbody>
<tr>
<td>Exp.</td>
<td>(0.321, 0.402)</td>
<td>(0.323, 0.400)</td>
</tr>
<tr>
<td>Simulation</td>
<td>(0.330, 0.409)</td>
<td>(0.349, 0.401)</td>
</tr>
</tbody>
</table>

**Reference:**
Case Studies Using UniMCO 4.0

Case Study 2: Microcavity OLED – Pure RGB Emissions

- Develop microcavity OLED
- Control cavity mode
- Control position of the resonance wavelength
- Narrow EL spectrum
- Enhance EL output
- Control EL directionality
- Obtain pure red, green, & blue color

<table>
<thead>
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<th>Devices</th>
<th>Layer thickness (nm)</th>
<th>Reference wavelength (nm)</th>
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<tr>
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<td>HTL</td>
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<td>80</td>
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<tr>
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<td>70</td>
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<td>90</td>
<td>70</td>
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</table>

<table>
<thead>
<tr>
<th>Devices</th>
<th>Layer thickness (nm)</th>
<th>Reference wavelength (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Red</td>
<td>162</td>
<td>80</td>
</tr>
<tr>
<td>Green</td>
<td>139</td>
<td>70</td>
</tr>
<tr>
<td>Blue</td>
<td>90</td>
<td>70</td>
</tr>
</tbody>
</table>
Case Studies Using UniMCO 4.0

Case Study 2: Microcavity OLED – Pure RGB Emissions

Compare with Exp:
• Match well with experimental data
• Slight deviation from experiment might be due to the experimental error of layer thicknesses

<table>
<thead>
<tr>
<th>CIE Color Coordinates of Microcavity Devices at Normal Direction:</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
</tr>
<tr>
<td>Experiment</td>
</tr>
<tr>
<td>Simulation</td>
</tr>
</tbody>
</table>

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Case Studies Using UniMCO 4.0

Case Study 2: Microcavity OLED – Pure RGB Emissions

Reference:
Case Study 3: Dual-Wavelength Bragg Reflectors (DWBR)

- Demonstrate dual-wavelength reflectivity bands
- Wide application in optoelectronic devices

- Reference wavelength = 1050 nm
- Each Q.W. GaAs layer = 75 nm
- Each Q.W. AlAs layer = 89 nm
- Set emitting layer (red)
- Set substrate (gray)
Case Studies Using UniMCO 4.0

Case Study 3: Dual-Wavelength Bragg Reflectors (DWBR)

Reference:
Case Study 4: Thickness Effect on EL of Polymer PPV OLED

- Thickness variation of MEH-DOO-PPV: 100, 86, 62, and 55 nm.

- Assumption: the emitting zone (red) is 5 nm thick and located at the center of the PPV layer

- The imaginary part of the refractive index of the PPV within the emitting zone is neglected because UniMCO requires the refractive index of the emitting layer be real

- From this example, the users show how to simulate the devices with a complex refractive index emitting layer.

Material Parameters:
- ITO: from UniMCO material database
- PEDOT-PSS: $n = 1.53$
- PPV: from the data file ppv_nk.txt
- Calcium: from the data ca_nk.txt
Case Study 4: Thickness Effect on EL of Polymer PPV OLED

Result Comparison:

The above results shows that the simulation results very closely match the experimentally determined spectra. Please note that the thickness of the ITO and the cathode material were not specified in the reference. Here we just pick the 50 nm as the ITO layer thickness and Ca as the cathode. These arbitrary choices might affect the simulation accuracy.

Reference:

UniMCO Can Do More…

UniMCO can be used to design, optimization, and simulate:

– LED and OLED
– Microcavity OLED
– Semiconductor RCLED
– VCSEL laser
– Optical multilayer film coating and optical filters
Why UniMCO?

Main features of UniMCO:

- UniMCO is easy to use
- UniMCO is a first ever commercial tool for MCOLED & RCLED
- UniMCO has the features that Microcavity LED and VCSEL designers need
- UniMCO has many features for modeling unusual microcavity designs including double-cavity (or RCR) structures
- UniMCO has powerful color-brightness simulation capabilities, which allow user to compare color and brightness between microcavity device and non-cavity device
- UniMCO provides a cost-effective solution