

# Multi-scale Dynamics of Organic Light-Emitting Devices

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Minnesota

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Dow Chemical for funding and collaboration. Dow scientists for research guidance, samples, etc.

# Dedication

To some people that I value

## Abstract

Over the last decade, organic light-emitting devices (OLEDs) have grown to receive tremendous attention for application in commercial displays and in lighting. While mostly successful for small format displays, challenges still exist that limit their performance for broader applications. Many of these limitations stem from a lack of understanding of charge and exciton dynamics and their impact on efficiency and stability. In this presentation, we describe novel device characterization and modelling efforts aimed at elucidating key dynamic processes in multiple regimes, including the microsecond transient behavior, steady-state, and long term degradation.

A model is presented which unifies both the transient and steady-state electroluminescence behavior of an OLED as a function of current density. The excellent agreement between the model and experiment enables a deeper understanding of efficiency reduction at high brightness. Additionally, the relatively ambiguous device efficiency parameter of charge balance is recast as an exciton formation efficiency. This framework permits a novel characterization paradigm for decoupling degradation pathways during OLED life-testing. In addition to the luminance loss, the degradation in emitter photoluminescence and exciton formation efficiency are also extracted. This technique is applied to an archetypical phosphorescent OLEDs, enabling more comprehensive design rules for device engineering to realize enhanced lifetime. Data science is a rising topic in industrial research. A system for enabling data science techniques within laboratory research is presented. Select useful applications are demonstrated.

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# 1 Overview of Organic Semiconductors

## 1.1 Organic Semiconductors

## 1.2 Excitons

### 1.2.1 Singlets and Triplets

### 1.2.2 Electronic Transitions

## 1.3 Charge Transport

## **2 Organic Light-Emitting Devices**

### **2.1 Fabrication Processes**

### **2.2 Characterization**

#### **2.2.1 Luminance**

#### **2.2.2 Efficiency Analysis**

### **2.3 Historical Development**

#### **2.3.1 The First OLEDs**

#### **2.3.2 Phosphorescence**

#### **2.3.3 Host-Guest Systems**

#### **2.3.4 Cohost Systems**

#### **2.3.5 Thermally Activated Delayed Fluorescence**

### **2.4 Device Operation**

#### **2.4.1 Dynamic Processes**

#### **2.4.2 Efficiency Roll-Off**



## 3 Transient and Steady-State Dynamics

### 3.1 Motivation

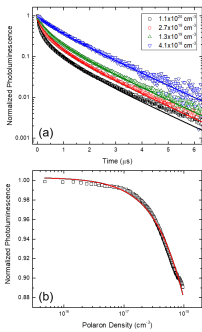
### 3.2 Theory

#### 3.2.1 Previous Efficiency Roll-Off Models

#### 3.2.2 Exciton Dynamics

#### 3.2.3 Polaron Dynamics

#### 3.2.4 Exciton Quenching in Photoluminescence



#### 3.2.5 Transient Electroluminescence

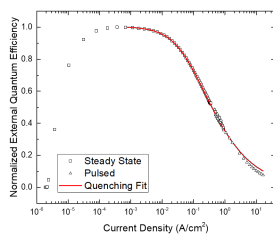
#### 3.2.6 Efficiency Analysis

### 3.3 Experimental Details

### 3.4 Application to Devices

#### 3.4.1 Overview of Approach

#### 3.4.2 Initializing Parameters with Quenching Only Steady-State Model



### 3.4.3 Transient Modeling

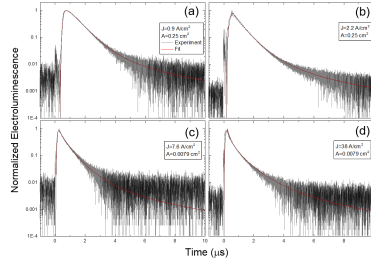
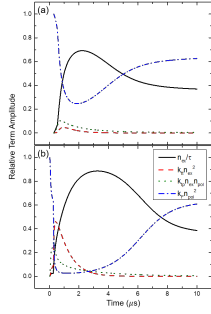


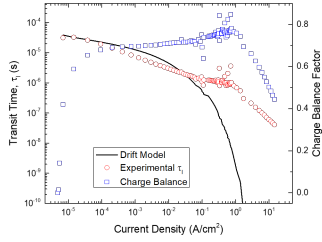
Table 1: Fit parameter extracted from transient and steady state electroluminescence. Transient EL fit parameters averaged over all measured current densities.  $\eta_{\text{EL}}$  Roll-off parameters averaged over several measured devices. Triplet-triplet annihilation and triplet-polaron quenching rates are fixed to those obtained from fitting the normalized efficiency roll-off.

	Transient EL	Efficiency Roll-off
$\tau$ (s)	$6.9 \pm 0.1 \times 10^{-7}$	$6.1 \times 10^{-7}$
$k_{\text{tr}}$ (cm <sup>3</sup> /s)	$7.1 \times 10^{-12}$	$7.1 \times 10^{-12}$
$k_{\text{tp}}$ (cm <sup>3</sup> /s)	$3.3 \times 10^{-13}$	$3.3 \times 10^{-13}$
$k_{\text{p}}$ (cm <sup>3</sup> /s)	$7.7 \pm 3.5 \times 10^{-12}$	$1.6 \times 10^{-11}$

### 3.4.4 Term Efficiency During Transient

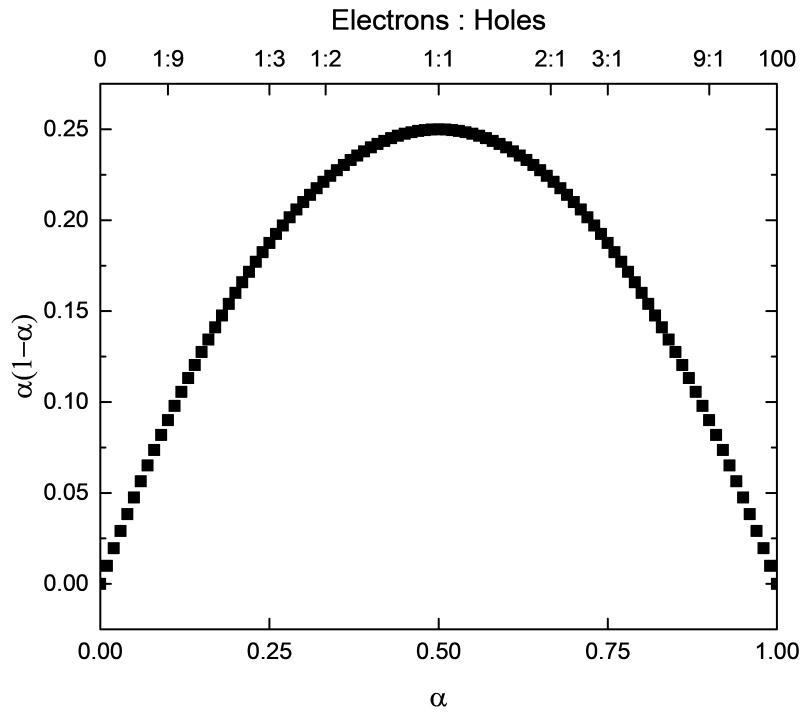
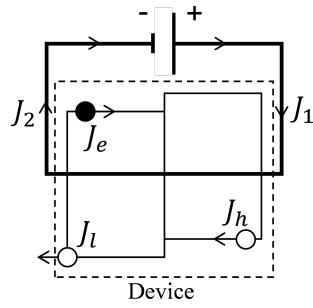


### 3.4.5 Extracting Exciton Formation Efficiency



### 3.4.6 Drift Model

## 3.5 Understanding Assumptions of Polaron Model



## 4 Integrated Photoluminescence Lifetimes

### 4.1 Luminance as Efficiency Loss

### 4.2 Photoluminescence Characterization

#### 4.2.1 Light Selection

#### 4.2.2 Absorption - Recombination Overlap

#### 4.2.3 Contact Degradation

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#### 4.2.5 Verification with Excton Lifetime

### 4.3 Experimental Implementation

#### 4.3.1 Hardware Setup

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#### 4.3.3 Database Integration

## 5 Applied Integrated Lifetimes

### 5.1 CBP Host Thickness

### 5.2 MEML Luminance Scaling

### 5.3 Dow Cohost

## **6 Novel Blue Emitter Developement**

### **6.1 Molecular Systems**

### **6.2 Performance Optimization**

### **6.3 Solution Molecular Aggregation**

## 7 Data Management for Devices

## 8 Modeling Out-Coupling

### 8.1 Theory

### 8.2 Recombination Zone Overlap During Lifetime



## 9 Future Research

## References

- [1] HERSHEY, K. W., AND COTTINGHAM, J. P. Material properties of pipes and reeds from the Southeast Asian khaen. *The Journal of the Acoustical Society of America* *129*, 4 (apr 2011), 2520–2520.
- [2] HERSHEY, K. W., AND HOLMES, R. J. Unified analysis of transient and steady-state electrophosphorescence using exciton and polaron dynamics modeling. *Journal of Applied Physics* *120*, 19 (2016), 195501.
- [3] HERSHEY, K. W., SUDDARD-BANGSUND, J., QIAN, G., AND HOLMES, R. J. Decoupling degradation in exciton formation and recombination during lifetime testing of organic light-emitting devices. *Applied Physics Letters* *111*, 11 (2017), 113301.
- [4] XU, F., HERSHEY, K. W., HOLMES, R. J., AND HOYE, T. R. Blue-Emitting Arylalkynyl Naphthalene Derivatives via a Hexadehydro-Diels-Alder Cascade Reaction. *Journal of the American Chemical Society* *138*, 39 (oct 2016), 12739–12742.

# Appendices

## A List of Publications

- HERSHEY, K. W., AND COTTINGHAM, J. P. Material properties of pipes and reeds from the Southeast Asian khaen. *The Journal of the Acoustical Society of America* 129, 4 (apr 2011), 2520–2520
- HERSHEY, K. W., AND HOLMES, R. J. Unified analysis of transient and steady-state electrophosphorescence using exciton and polaron dynamics modeling. *Journal of Applied Physics* 120, 19 (2016), 195501
- HERSHEY, K. W., SUDDARD-BANGSUND, J., QIAN, G., AND HOLMES, R. J. Decoupling degradation in exciton formation and recombination during lifetime testing of organic light-emitting devices. *Applied Physics Letters* 111, 11 (2017), 113301
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## B Out-Coupling Code

## C Lifetime Box Code

## D List of Figures

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