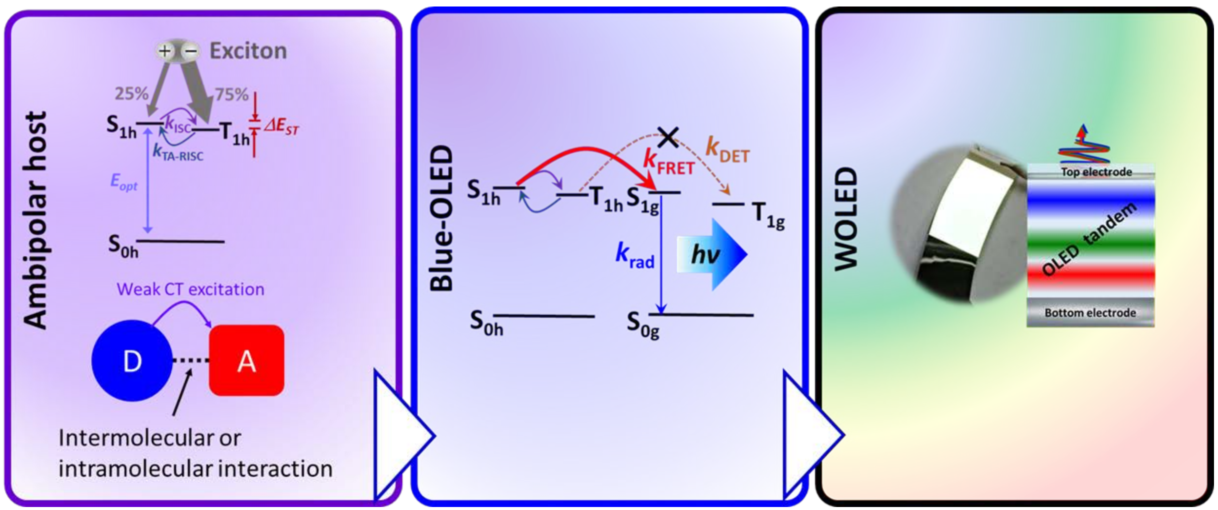
U.S. DEPARTMENT OF ENERGY

Office of ENERGY EFFICIENCY & RENEWABLE ENERGY

Stable White Organic Light-Emitting Diodes Enabled by New Materials with Reduced Excited-State Lifetimes



Georgia Tech Research Corporation

PI: Professor Bernard Kippelen

PI Tel. 404-385-5163 / Email: bernard.kippelen@ece.gatech.edu

Project Summary

Timeline: New Project

Start date: Sep. 1, 2017 Planned end date: Aug. 31, 2019

Key Milestones (Budget period 1)

1. Milestone 1; Ambipolar hosts with a wide optical bandgap (E_{opt} > 2.7 eV) and (ΔE_{ST} < 0.3 eV). (09/2018)
2. Milestone 2; blue OLEDs that achieve PE values larger than 40 lm/W with efficiency roll-off (ca. 20%). (09/2018)

Budget:

Total Project $ to Date (03/31/2018):

- DOE: $233,540
- Cost Share: $74,382

Total Project $:

- DOE: $896,000
- Cost Share: $224,000

Key Partners:

Seth Marder	
Jean-Luc Bredas	

Project Outcome:

The proposed theoretical and experimental program aims at developing blue-emissive layers that display simultaneously near 100% internal quantum efficiency (IQE) *and* short excited-state lifetimes to overcome the existing efficiency vs. stability tradeoff displayed by blue-emitting OLEDs and by WOLEDs, and to demonstrate stable WOLEDs that fulfill or exceed the 2020 target metrics (RDP 2016 section C.1.2) ahead of schedule

Team

Two decades of collaboration in the field of organic electronics and photonics:

- Industry-funded projects
- NSF (STC-MDITR)
- DOE (EFRC-CISSEM)
- DoD (multiple MURI)

Georgia Tech School of Electrical and Computer Engineering, College of Engineering

Characterization of optoelectronic properties of materials and device fabrication, simulation and characterization

State-of-the-art facilities and equipment to fabricate and characterize materials and OLEDs.

Prof. Bernard Kippelen, PI
Internationally recognized expert in organic electronics and in the design, fabrication and characterization of OLEDs in particular

Dr. Canek Fuentes-Hernandez

Prof. Seth Marder, Co-PI
Internationally recognized expert in the synthesis of conjugated molecules and polymers for organic electronics.

Dr. Stephen Barlow

Design and synthesis of low-ΔE_{ST} host and emitter materials based on intramolecular D-A approach and components of intermolecular host approach as required:

State-of-the-art facilities and equipment for synthesizing, purifying, and characterizing organic and organometallic materials.

Georgia Tech Chemistry and Biochemistry, College of Sciences

Prof. Jean-Luc Brédas, Co-PI
Internationally recognized expert in modeling based on density functional theory methodologies and molecular dynamics simulations.

Theoretical design of new TADF molecular architectures and description of their electronic structure:

Access to the Center for Computational Molecular Science and Technology at GA Tech and supercomputers at national supercomputing resource centers through independent research grants from the US Department of Defense

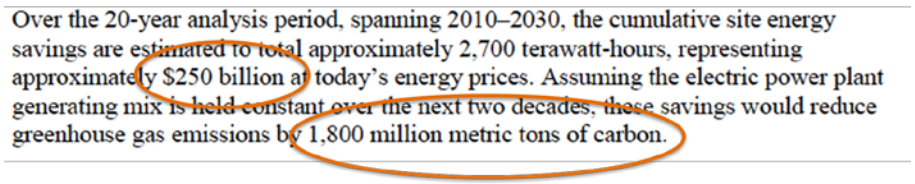
Dr. Veaceslav Coropceanu

Challenge


U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy

BUILDING TECHNOLOGIES PROGRAM

Energy Savings Potential of Solid-State Lighting in General Illumination Applications

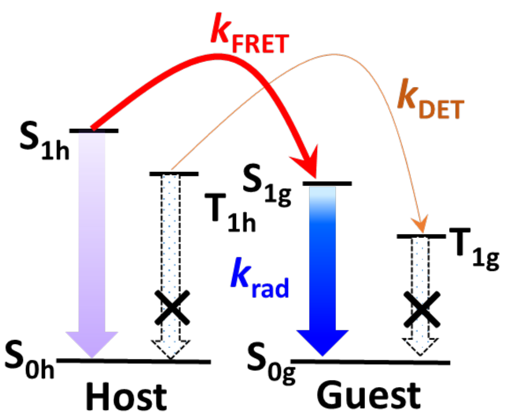

Over the 20-year analysis period, spanning 2010–2030, the cumulative site energy savings are estimated to total approximately 2,700 terawatt-hours, representing approximately $250 billion at today's energy prices. Assuming the electric power plant generating mix is held constant over the next two decades, these savings would reduce greenhouse gas emissions by 1,800 million metric tons of carbon.

Challenge: long-lived excited states in organic lumophores lead to the formation of higher energy states (> 4.3 eV) through up-conversion processes that are responsible for material degradation (e.g. bond cleavage).

Opportunity: harvest all excited states through thermally activated delayed fluorescence (TADF) to get 100% internal efficiency and transfer energy through FRET to fluorescent dopant to shorten lifetime and reduce degradation through up-conversion and roll-off of efficiency under high injection.

Challenge

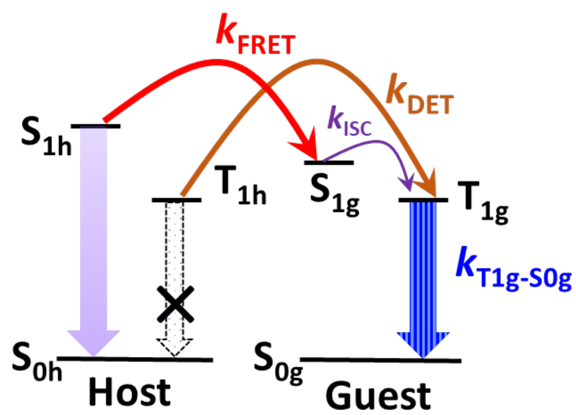
Fluorescence



- Max. IQE = 25%
- Max. EQE ca. 6% due to out coupling losses

- Long-term stability

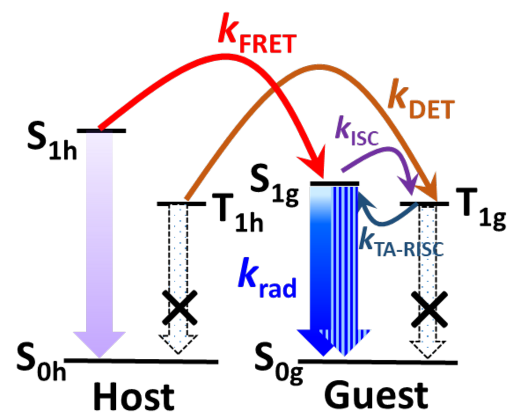
Phosphorescence



- Max. IQE = 100%
- Max. EQE ca. 25% due to out coupling losses

- Poor long-term stability

Thermally activated delayed fluorescence

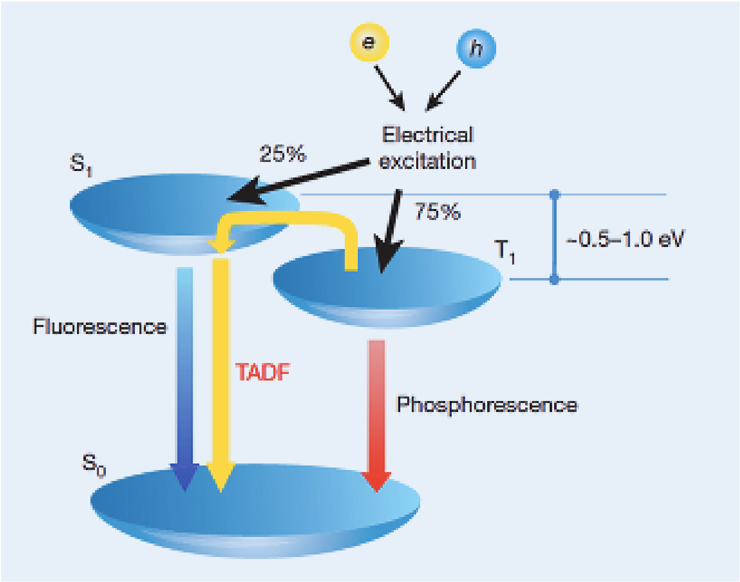


- Max. IQE = 100%
- Max. EQE ca. 25% due to out coupling losses

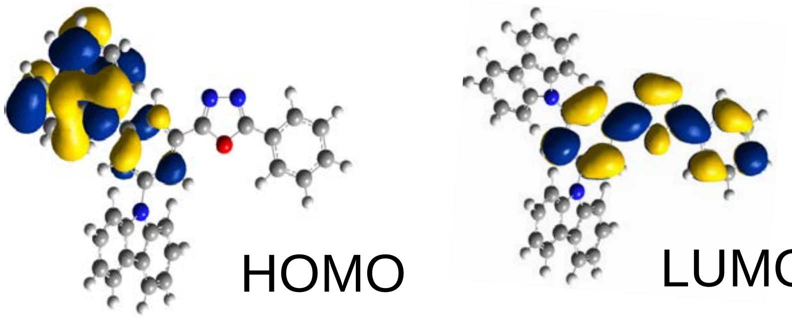
- Poor long-term stability

Approach: Thermally Activated Delayed Fluorescence

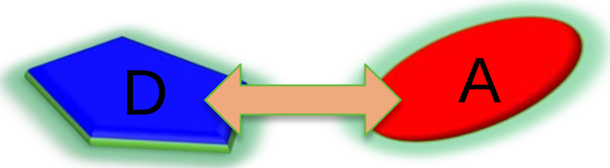
All-organic compounds that do not contain precious heavy metals, an alternative to phosphorescence



Key metric: ΔE_{ST}



New design criteria based on coupling of donor and acceptor-like moieties.

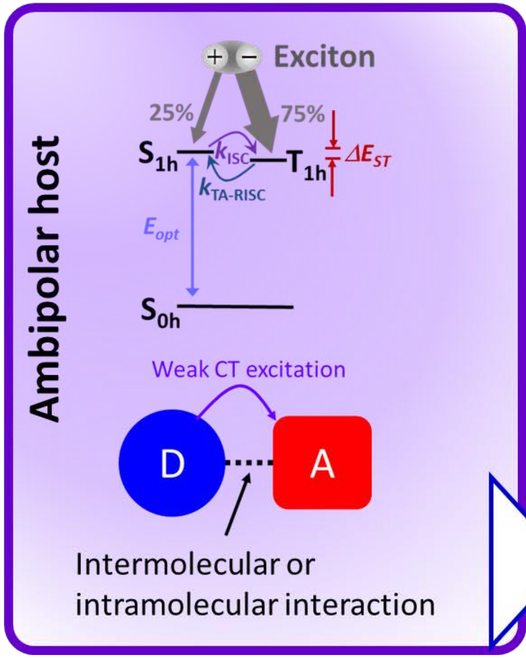


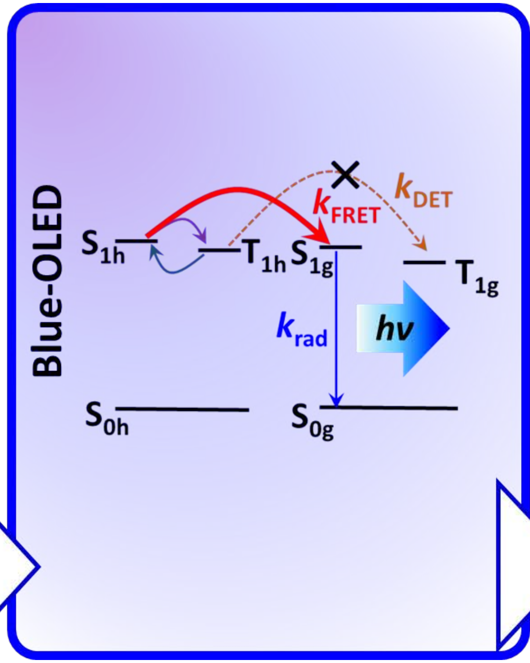
Intramolecular and **inter**molecular

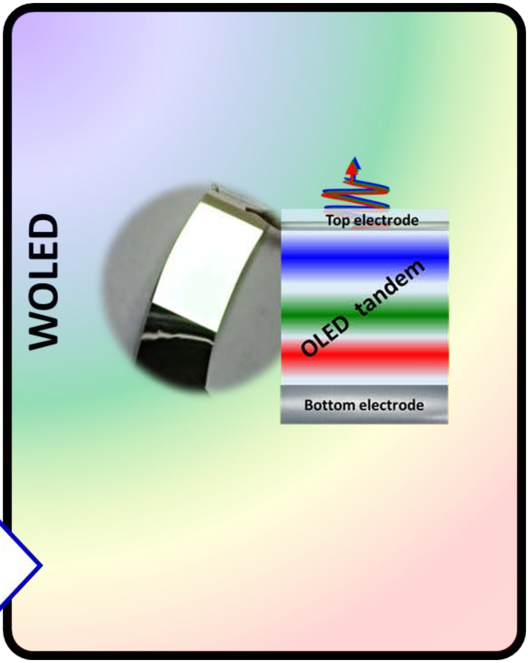
Uoyama, H., Goushi, K., Shizu, K., Nomura, H., Adachi, C. *Nature*. 492, 234 (2012).
Nakanotani, H., Masui, K., Nishide, J., Shibata, T., Adachi, C., *Scientific Reports*. 4, 2127 (2013).

Approach

Overcome existing device efficiency vs. device stability tradeoff in blue-emitting OLEDs to enable next-generation stable white OLEDs (WOLEDs).







Emission

- Fluorescence (F): Efficient FRET to S_{1g} and fast decay to S_{0g}

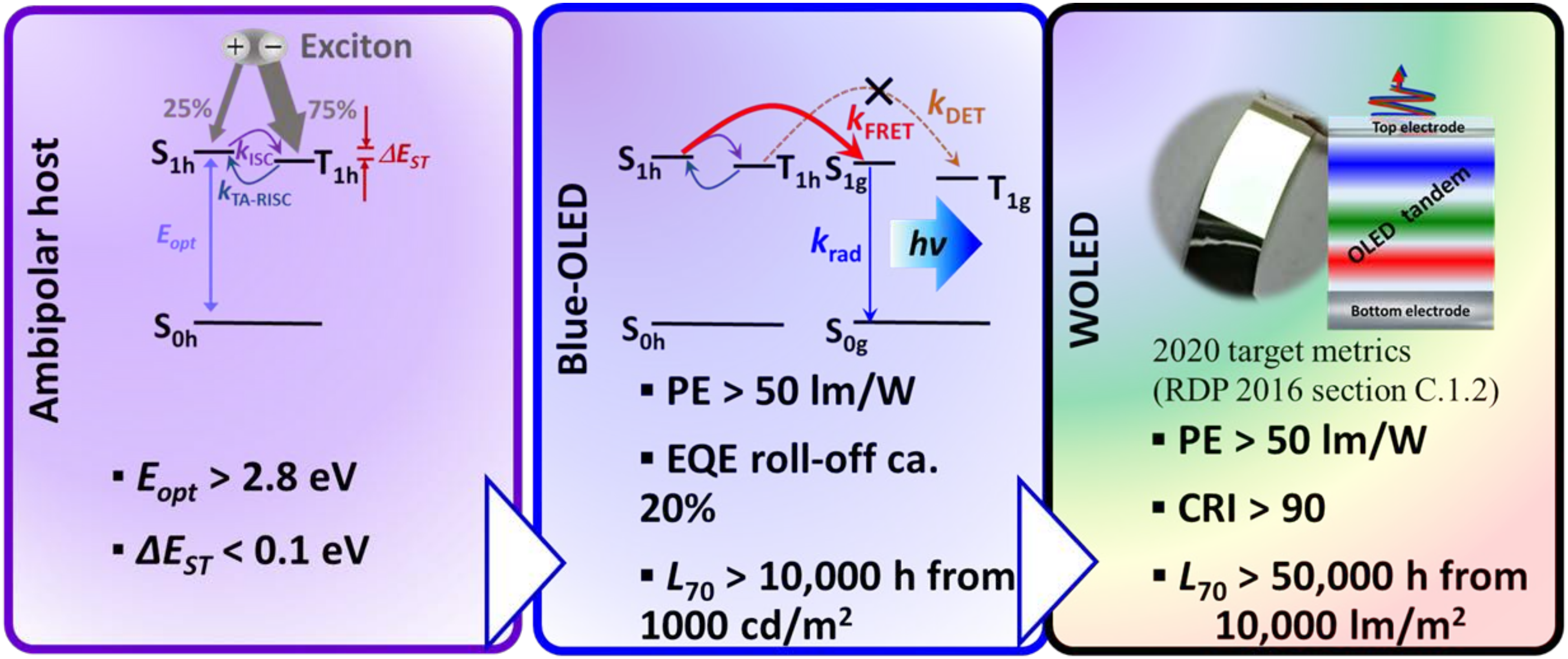
- Max. IQE = 100%
- $k_{rad} < 10^5$ s^{-1} (short-lived excited states)

- Maximum EQE ca. 25-40% due to out coupling losses
- Low excited state density

- Small EQE roll-off
- Reduced exciton annihilation rate

- Long-term stability

Impact



The proposed emissive layers will be all-organic and comprise molecules typically synthesized in a few steps in high yields. We expect the device performance and cost of materials developed in this program to be in alignment with the 2020 target metrics and goals of DOE's SSL program for OLED technology.

Progress

Early stage: Q1 and Q2 emphasis is on material R&D

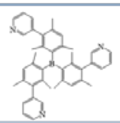
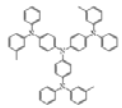
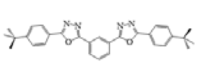
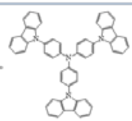
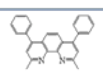
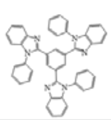
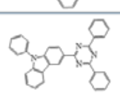
Goal #1
Wide-bandgap ambipolar hosts

- **Task 1.1** Wide-bandgap ambipolar low ΔE_{ST} D:A intermolecular host
- **Task 1.2** Wide-bandgap ambipolar low ΔE_{ST} D-A intramolecular host

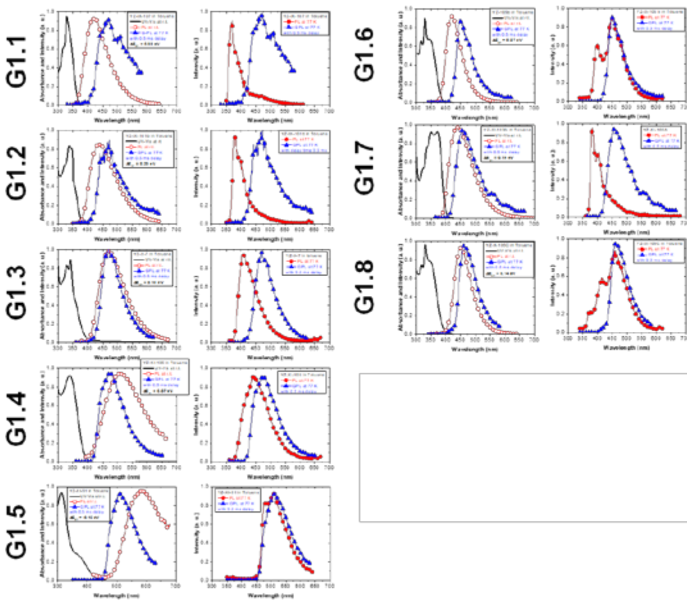
Goal #2
Blue-OLEDs

- **Task 2.1** Blue OLEDs

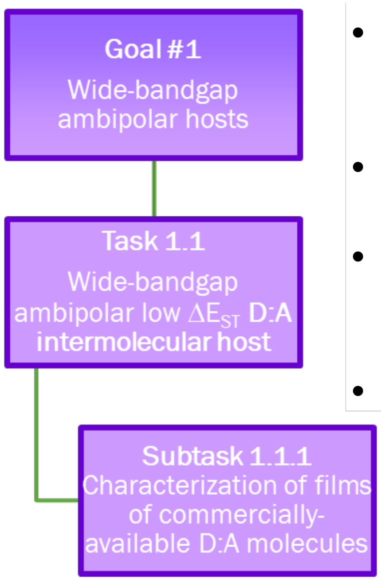
Selected & characterized intermolecular hosts (Q1.Milestone)

	Acceptor		Donor
	**3TPYMB**, Tris(2,4,6-triMethyl-3-(pyridin-3-yl)phenyl)borane		**m-MTDATA**, 4,4′,4″-tris (3-methylphenylphenylamino) triphenylamine
	**OXD-7**, 1,3-bis[2-(4-tert-butylphenyl)-1,3,4-oxadiazo-5-yl]-benzene		**TCTA**, tris(4-carbazoyl-9-ylphenyl)amine
	**BCP**, 2,9-dimethyl-4,7-diphenyl-1,10-phenanthroline		**TCTA**
	**TPBi**, 2,2′,2″-(1,3,5-benzinetriyl)-tris(1-phenyl-1-H-benzimidazole)		**TCTA**
	**DPTPCz**, 3-(4,6-diphenyl-1,3,5-triazin-2-yl)-9-phenyl-9H-carbazole		**TCTA**

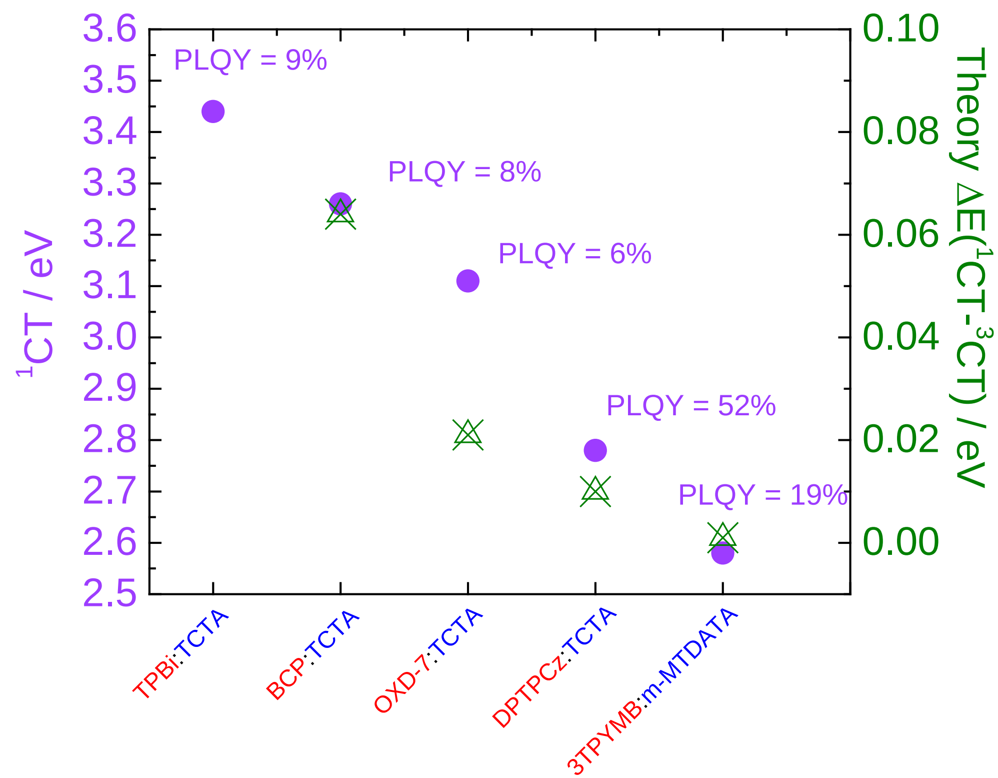
Synthesized & characterized 1-gen intramolecular hosts (Q2. Milestone)



Progress

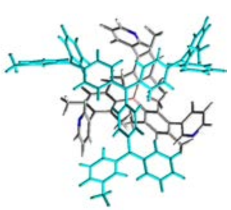


- Selected, acquired and purified D and A materials
- Prepared films by co-evaporation
- Film characterization: PL, PLQY, refractive index, etc. (in progress)
- Conducted computational studies (in progress)

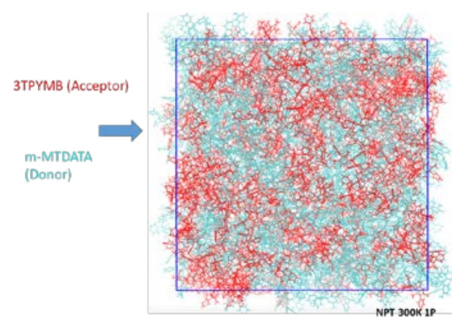


Progress aligned with goals and objectives in the SOW

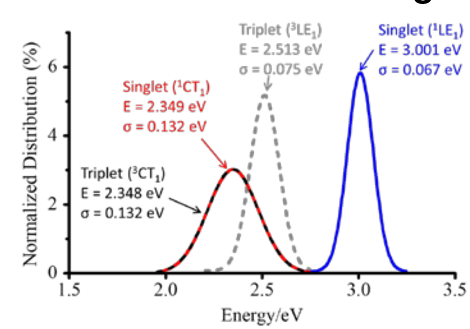
Structure:



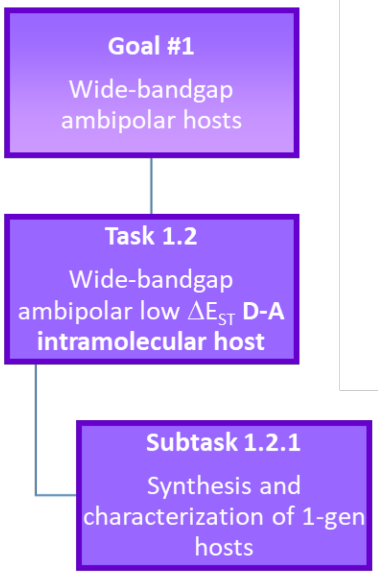
Morphology:



Distribution of state energies:

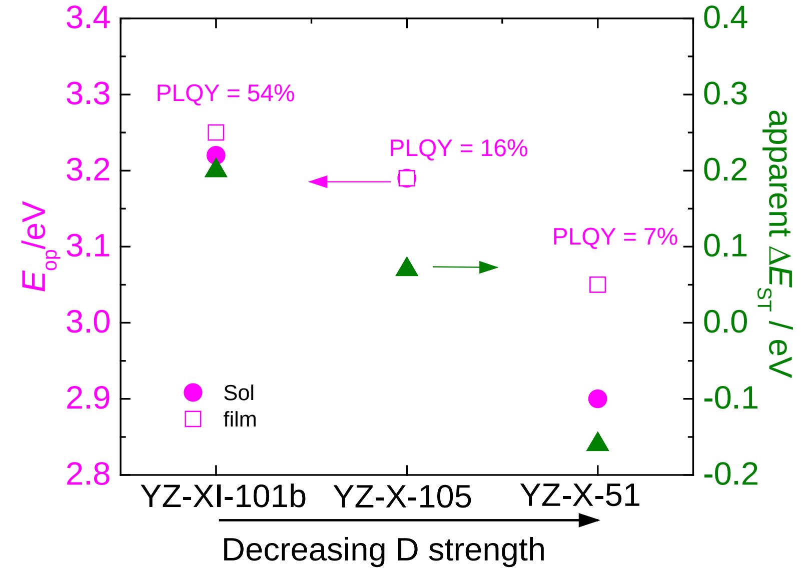


Progress

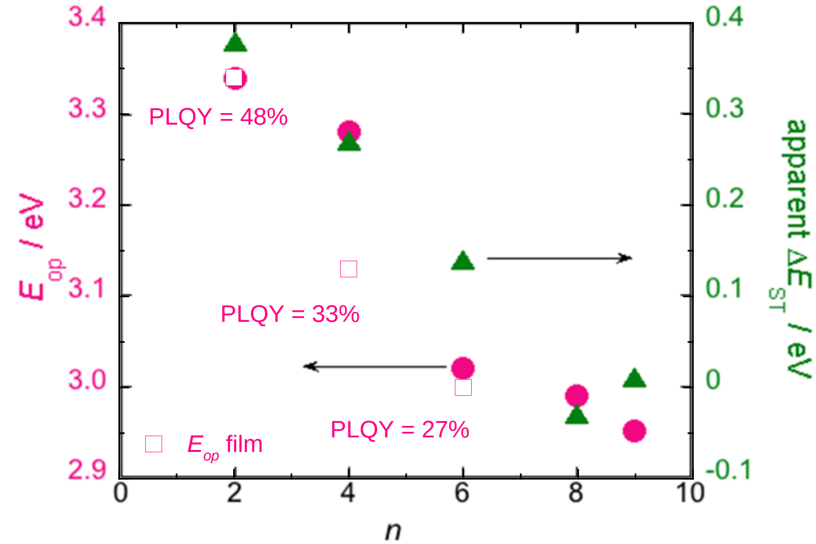


- Synthesized 1-gen intramolecular hosts
- Prepared solutions and films by co-evaporation
- Solution and film characterization: PL, PLQY, refractive index, etc. (in progress)

Series showing effect of decreasing D strength



Series showing effect of number of carbazoles (*n*)



Progress aligned with goals and objectives in the SOW

Progress

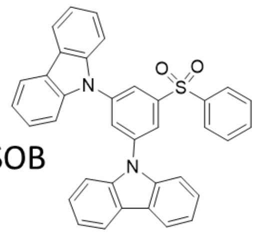
Goal #2
Blue-OLEDs

Task 2.1 Blue OLEDs

Subtask 2.1.1
Blue emissive layer

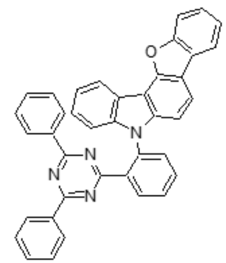
- Scale up of mCPSOB
- Initial selection of emitters /hosts and characterization

mCPSOB

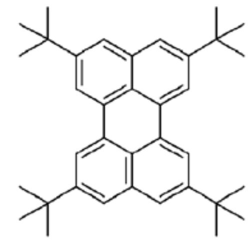


E_S = 2.93 eV
E_T = 3.02 eV
ΔE_{ST} = 90 meV

Emitter

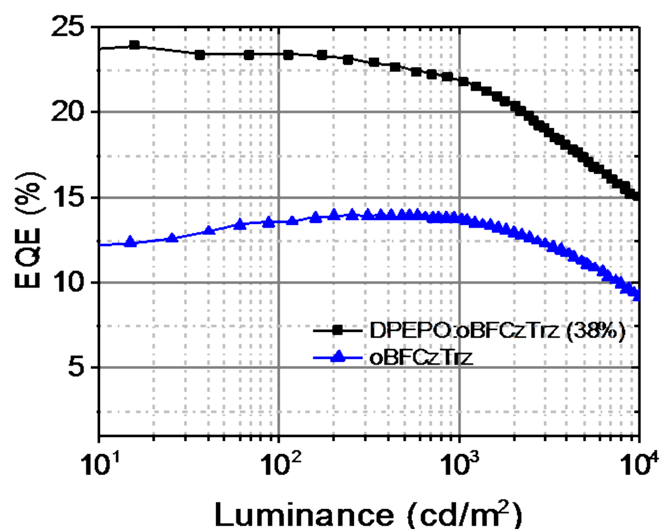


oBFCzTrz
ΔE_{ST}=0.002 eV [1]
Lee, Dong Ryun, et al. *ACS Appl. Mat. & Inter.* 8.35 (2016): 2319.



TBPe

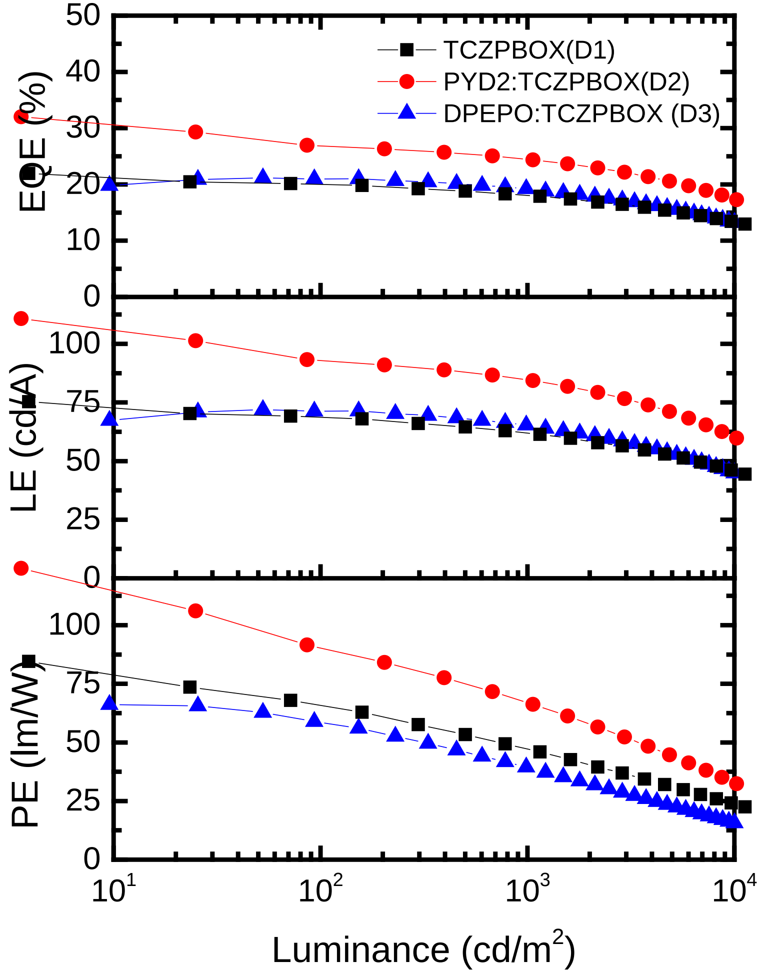
Progress on schedule. Other emitters are currently being considered based on PL characterization of host

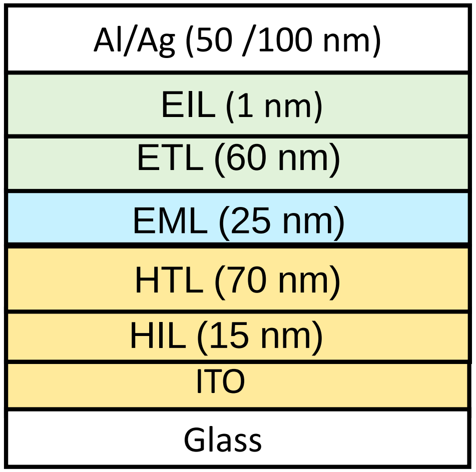


Example of past results on blue TADF emitting devices

Progress

Recent results towards the validation of the project's approach





Heavy metal-free neat and doped TADF emitters can lead to OLEDs with high efficiency. EQE = 24.4% @ 1,000 cd/m^2 (green color).

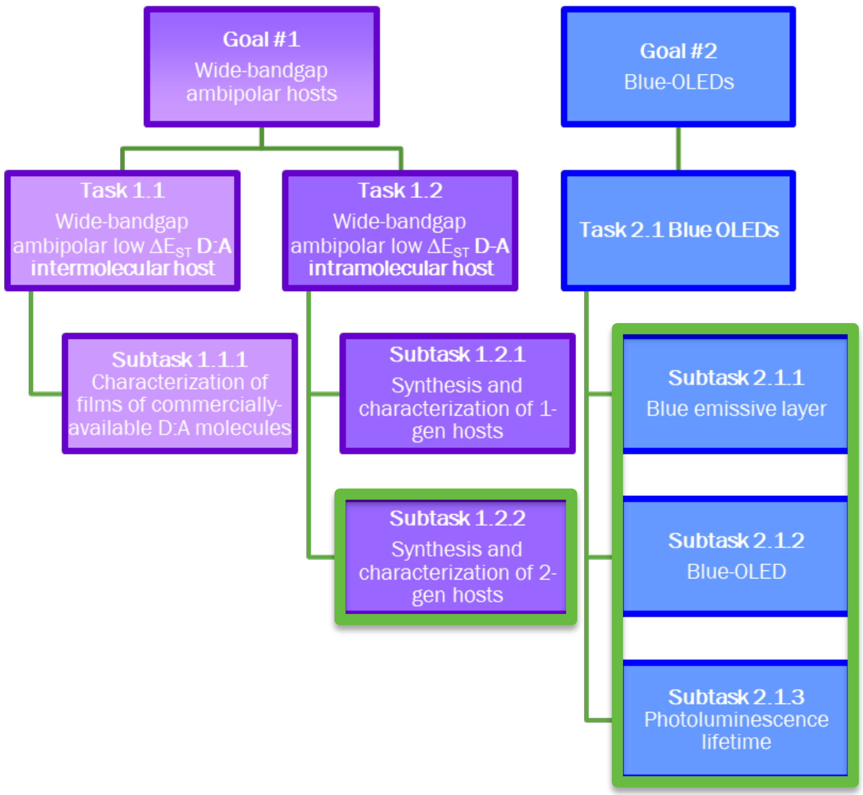
Stakeholder Engagement

Early stage:

- Six joint group meetings have been held to review progress
- Weekly interactions between research scientists and students, to conduct experiments and to exchange materials and results
- PI and research scientist attended DOE SSL Workshop in Nashville.
- PI attended OLED Stakeholder meeting hosted by 3M and presented
- PI and Co-PIs have plans to attend conferences such as SPIE and MRS
- The Marder and Kippelen groups, with funding from the Mitsubishi Chemical Group are collaboratively developing blue-emitting OLEDs for display applications.

Remaining Project Work

Budget Period 1



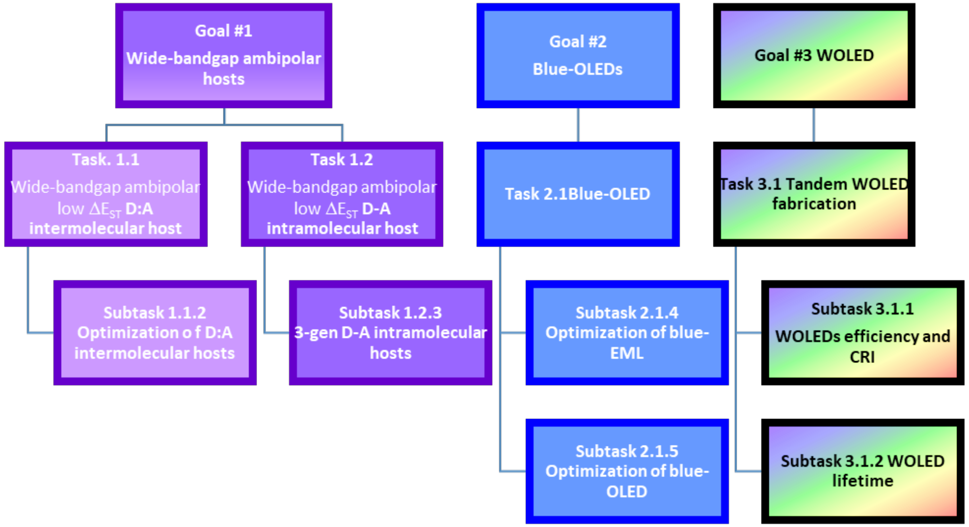
Q1	Commercial D and A Molecules Acquired Task 1.1	Technical	Acquisition and purification of selected D and A molecules completed
Q2	D:A host Films Characterized and Selected Task 1.1	Technical	D:A intermolecular host films with $E_{opt} > 2.5$ eV and $\Delta E_{ST} < 0.3$ eV
Q2	Synthesis of 1-gen D-A Intramolecular Host Molecules Task 1.2	Technical	1-gen D-A intramolecular compounds with $E_{opt} > 2.5$ eV and $\Delta E_{ST} < 0.3$ eV
Q3	Synthesis of 2-gen D-A Intramolecular Host Molecules Task 1.2	Technical	2-gen D-A intramolecular compounds with $E_{opt} > 2.6$ eV and $\Delta E_{ST} < 0.3$ eV
Q3	1-gen Blue-OLED demonstration Task 2.1 Q3	Technical	OLEDs using 1-gen blue emissive layers (EML) with PE > 20 lm/W
Q4	Intermolecular Host Films Characterized Task 1.1	Go/No Go	D:A intermolecular host film with $E_{opt} > 2.7$ eV and $\Delta E_{ST} < 0.3$ eV demonstrated
Q4	Intramolecular Host Compounds Characterized Task 1.2	Go/No Go	D-A intramolecular compounds with $E_{opt} > 2.7$ eV and $\Delta E_{ST} < 0.3$ eV demonstrated
Q4	Blue-OLED Demonstrated Task 2.1	Go/No Go	B-OLEDs PE > 40 lm/W; EQE roll-off ca. 20%

We are here.

Blue –OLED work will start in Q3

Remaining Project Work

Budget Period 2



Q5	Intermolecular Guest/Host Demonstrated Task 1.1 Q5	Technical	D:A intermolecular host with E_{opt} > 2.8 eV and ΔE_{ST} < 0.1 eV
Q5	3-gen D-A Intramolecular Films Characterized and Selected Task 1.2 Q5	Technical	3-gen D-A intramolecular films with E_{opt} > 2.8 eV and ΔE_{ST} < 0.1 eV
Q6	Blue Guest-host Emitter Layer Optimized Task 2.1 Q6	Technical	D:A or D-A host with E_{opt} > 2.8 eV and ΔE_{ST} < 0.1 eV with 80% efficient FRET transfer to dopant and excited-state lifetime < 1 μs
Q6	Blue OLEDS Demonstrated Task 2.1 Q6	Technical	Blue OLEDs with PE > 50 lm/W and EQE roll-off ca. 20% and $L_{70\%}$ >10,000 h at 1,000 cd/m^2
Q7	Tandem WOLEDS CRI Values Characterized Task 3.1 Q7	Technical	Tandem WOLEDs with PE values larger than 50 lm/W. Tandem WOLEDs with CRI values larger than 90;
Q8	Tandem WOLEDS Outputs Characterized Task 3.1 Q8	Technical	Tandem WOLEDs with L_{70} larger than 50,000 h from an initial light output of 10,000 lm/m^2;

Thank You

Georgia Tech Research Corporation

PI: Professor Bernard Kippelen

PI Tel. 404-385-5163 / Email: bernard.kippelen@ece.gatech.edu

REFERENCE SLIDES

Project Budget

Project Budget: New project started Sep. 1, 2017.
Variances: None
Cost to Date: **As of 3/31/2018, DOE: $233,540; Cost-share: $74,382**
Additional Funding: NA

Budget History					
New project start date: Sep. 1, 2017		FY 2018 (current) Budget period 1		FY 2019 – Aug. 31, 2019 (planned budget period 2)	
DOE	Cost-share	DOE	Cost-share	DOE	Cost-share
$233,540	$74,382	$443,536	$110,884	$452,464	$113,116

Project Plan and Schedule

	Stable White Organic Light-Emitting Diodes Enabled by New Materials with Reduced Excited-State Lifetimes	FY2018				FY2019			
		Q1 (Oct-Dec)	Q2 (Jan-Mar)	Q3 (Apr-Jun)	Q4 (Jul-Sep)	Q5 (Oct-Dec)	Q6 (Jan-Mar)	Q7 (Apr-Jun)	Q8 (Jul-Sep)
Goal #1. Wide bandgap ambipolar hosts	**Task 1.1 Wide-bandgap low-ΔE_{ST} ambipolar D:A intermolecular host**								
	Subtask 1.1.1 - Characterization of films of commercially-available D:A molecules								
	* Acquisition and purification of commercially-available D and A molecules								
	* Characterization of relevant optical and electrical properties								
	* Computational studies								
	Subtask 1.1.2 Optimization of D:A intermolecular hosts								
	* Synthesis and characterization of optimized D:A intermolecular hosts								
	* Computational studies								
	Task 1.2 Wide-bandgap low-ΔE_{ST} ambipolar D-A intramolecular hosts								
	Subtask 1.2.1 Synthesis and characterization of 1-gen hosts								
	* Synthesis and chemical characterization								
	* Characterization of films								
	Subtask 1.2.2 Synthesis and characterization of 2-gen hosts								
	* Synthesis and chemical characterization								
	* Characterization of films								
	* Computational studies								
	Subtask 1.2.3 3-gen D-A intramolecular hosts								
	* Synthesis and chemical characterization								
	* Characterization of films								
	* Computational studies								
Goal #2. Blue OLEDs	**Task 2.1 Blue organic light emitting diodes (OLED)**								
	Subtask 2.1.1 Blue emissive layer (EML)								
	* Scaleup mCPSOB								
	* Selection of guest emitters and characterization of EMLs								
	* Computational studies								
	Subtask 2.1.2 Blue OLED								
	* Fabrication and optimization of blue-OLED								
	Subtask 2.1.3 Photoluminescence lifetime								
	* Photoluminescence lifetime stidies								
	Subtask 2.1.4 Optimization of blue Emissive Layer (EML)								
	* Fabrication and optimization of blue-OLED								
	* Lumen maintenance studies								
	Subtask 2.1.5 Optimization of blue OLED								
	* Fabrication and optimization of blue-OLED								
	* Lumen maintaince experiments								
Goal #3. WOLEDs	**Task 3.1 Tandem white organic light emitting diodes (WOLED)**								
	Subtask 3.1.2 WOLED EQE and CRI								
	* Scale up of relevant materials								
	* Modeling, fabrication and optimization of EQE and CRI of WOLED								
	Subtask 3.1.2 WOLED lifetime								
	* Optimization of WOLED lifetime								
	Task 4. Reporting and dissemination								
	Task 5. All activities related to managing the program								

Milestone ◇ Go/No-go decision △ Detailed briefings □ Annual report ◇ | Kippelen | Marder | Bredas

Filled symbols & areas = Completed