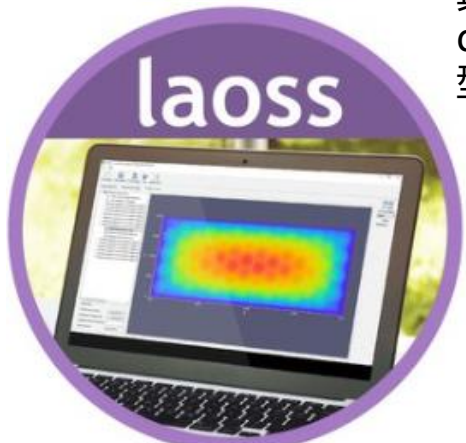


# SPI solutions

- Setfos+Laoss/Paios+Phelos
- Integration 无缝整合独特功能!
- All Pero Tandem Solar Cell
- TADF based OLED

# FLUXiM

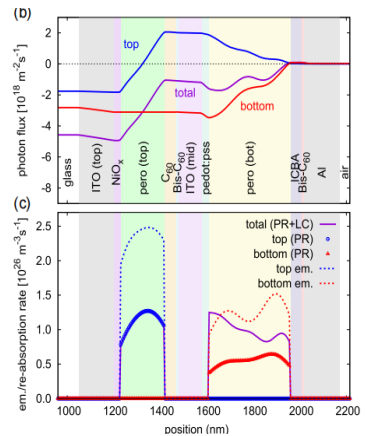
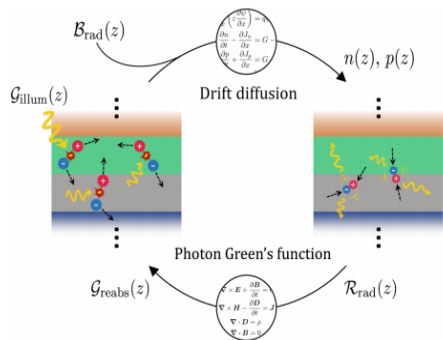
<https://www.fluxim.com>



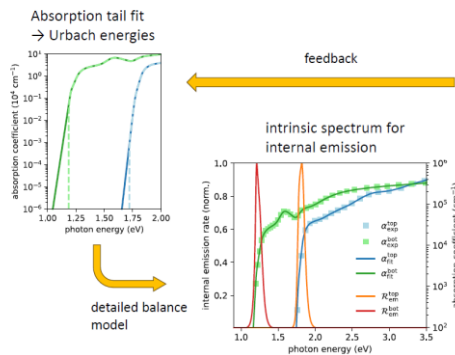
钙钛矿Perovskite(Pero)薄膜光电器件具备极大市场应用潜力和有望大幅提升性能, 如钙钛矿光伏优化QFLs/Voc增加, LED光子再利用PR/EQE提高。

FLUXiM在欧盟SuPerTandem/MUSICODE研究项目下,基于偶极子Dipole emission模型,电磁波格林函数Green Function和包括Scattering, Ray Tracing等多尺度模型,利用Setfos/Laoss模拟仿真软件,充分考虑光子Dipole取向, secondary generation. re-distribution/re-absorption 提出全钙钛矿Tandem solar cell新型光电产生机制:

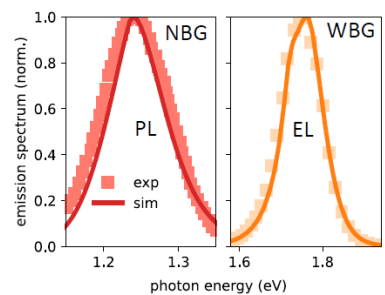
- Photon Recycling (PR)
- Luminescent Coupling(LC)



Cell level model parameters - optical



Fit of PL/EL spectrum  $\rightarrow$  peak energies and FWHM



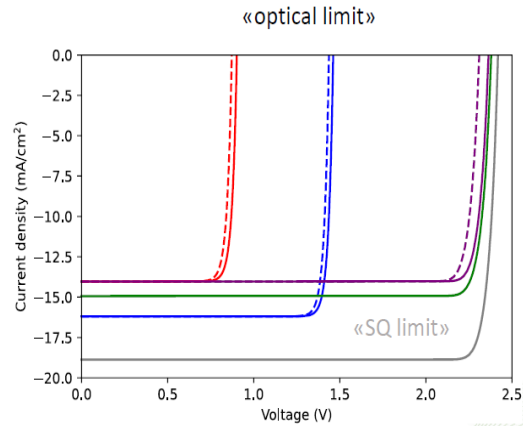
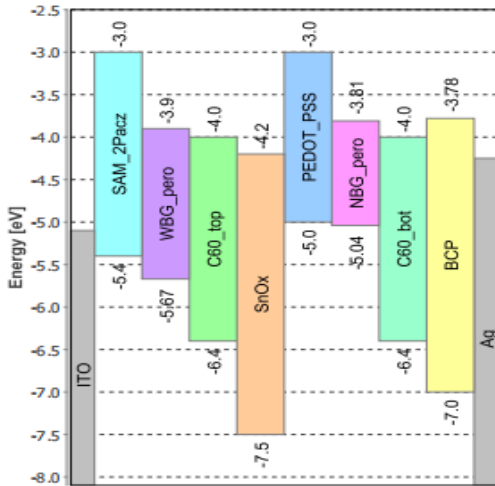
dipole radiation model



# Solutions & Applications: SuPerTandem

**SuPerTandem 目标:** 32% PCE on small area Cell, >30% Module efficiency (>100 cm<sup>2</sup>), 同时模拟分析模组遮挡和不同移动离子浓度下的反向电压/击穿Breakdown.

## Cell Model



- Ideal transport (flat QFLs)
- Electrically loss-free interconnect (no voltage drop)
- Explicit photon recycling and luminescent coupling within detailed balance

### optical simulation

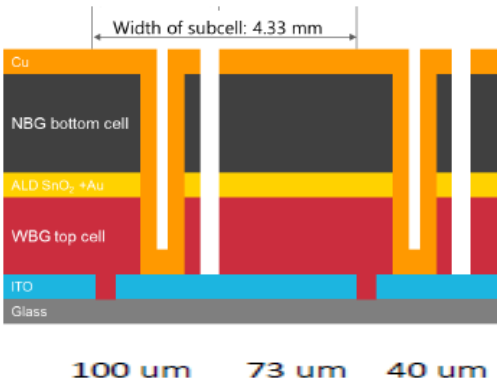
- TMM for coherent optics
- Ray-tracing for scattering
- Photon recycling & luminescent coupling

### electrical simulation

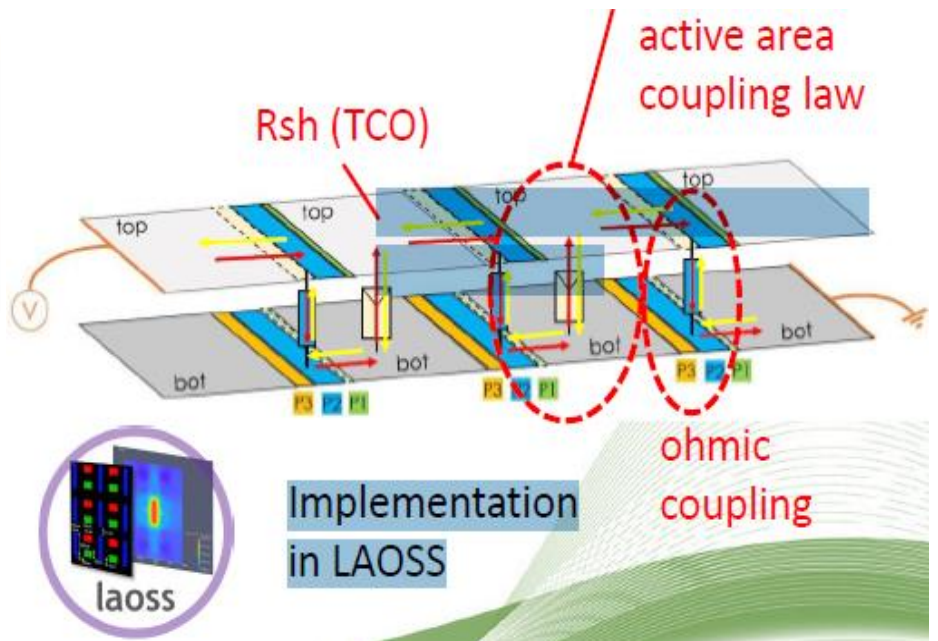
- Drift-diffusion-Poisson
- Mobile ions
- Bulk & interface defects
- Recombination junction



## Module Model

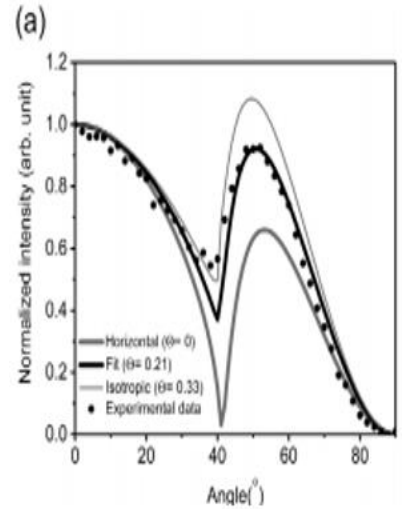
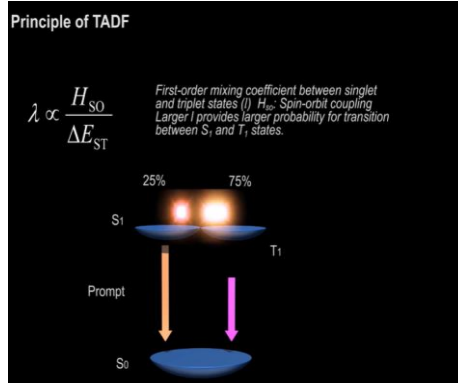
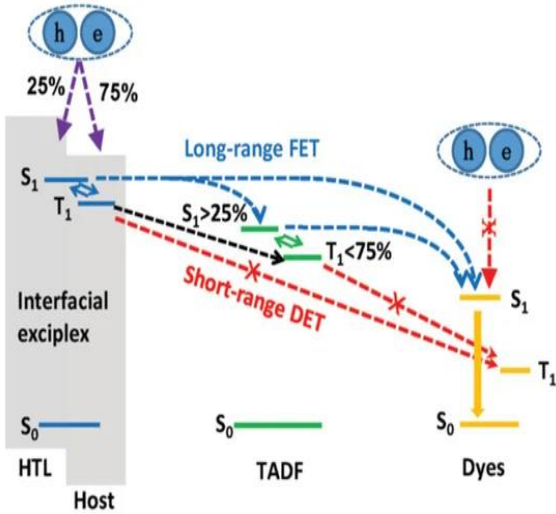


dead area width (WDA)



# Solutions & Applications:

## TADF- based OLED



A Boron, Nitrogen, and Oxygen Doped  $\pi$ -Extended Helical Pure Blue Multiresonant Thermally Activated Delayed Fluorescent Emitter for Organic Light Emitting Diodes That Shows Fast **k<sub>RISC</sub>** Without the Use of Heavy Atoms

九州大学Prof.C.Adachi 2024年文章中指出: TADF 工作机制 $\Delta E_{ST}$ 减小,同时也应满足 Spin Orbit Coupling(SOC) 和  $k_{RISC}/k_s$  条件, 如此也改进TTA/TPQ效能滚降(Roll-off) 问题和得到更窄FWHM 24nm深蓝光的MR-TADF for Rec.BT.2020-2标准。Setfos可以模拟Emitter TDM(Transition Dipole Moments)提取Host分子水平取向说明增强光输出耦合。

MR-TADF之外,TSCT(Through-Space Charge-Transfer) TSF/PSF/DSF-TADF OLED 均能以 Setfos 模拟:

3D Excitonic Master Equation, Rad/Non-Rad decay rate, TTA/TPQ,  $k_{RISC}/k_{ISC}/k_s/k_T$ , Foster transfer/Dexter radius, Low to high energy transfer/TADF.....



Screenshot of the Setfos software interface showing the Excitons tab. It displays various parameters for exciton generation, decay rates, and energy transfer rates.

Screenshot of the Setfos software interface showing the 3D Excitonic Master-Equation tab. It displays parameters for material properties, generation efficiency, and decay rates.

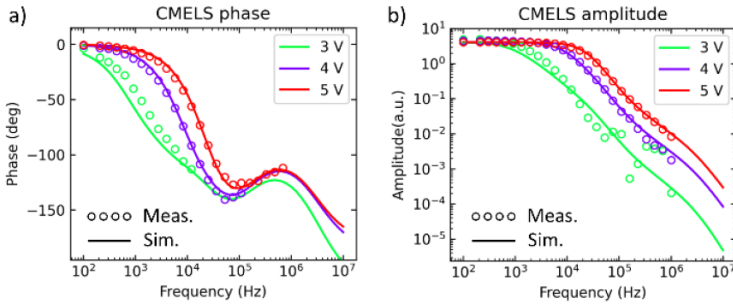


# Solutions & Applications:

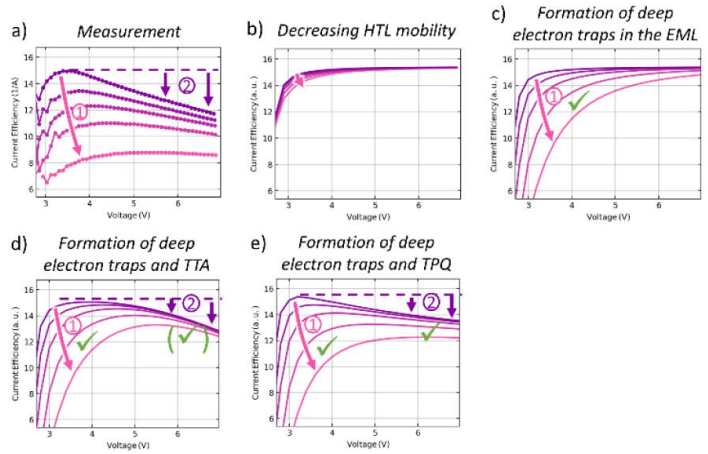
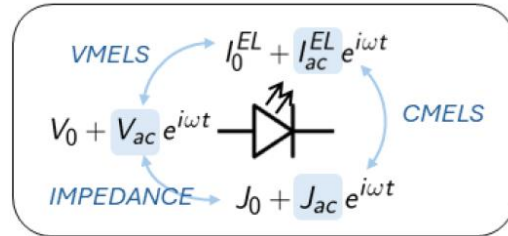
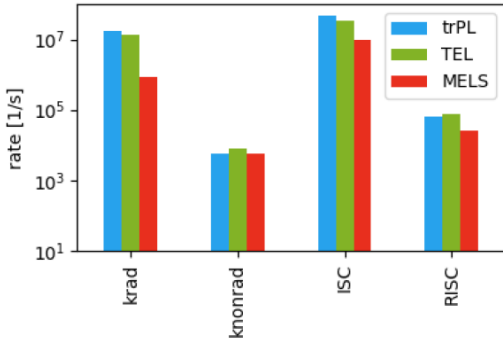
## Modulated EL Spectroscopy for exciton dynamics and degradation analysis for TADF OLED:

Exciton Dynamics and Degradation Mechanism in TADF OLEDs assessed by Modulated Electroluminescence Spectroscopy

B. Blülle\*, S. Jenatsch\*, H. Carrillo-Núñez\*, S. Züfle\*, B. Ruhstaller\*\*  
 \*Fluxim AG, Winterthur, Switzerland  
 \*\*ZHAW Zurich University of Applied Sciences, Switzerland



Setfos model fit of the spectral CMELS phase (a) and amplitude (b) for varying bias voltage.



a) Measured time evolution of the current efficiency vs. voltage and the corresponding Setfos model for potential quenching and degradation mechanisms (b – e). A good qualitative agreement is obtained, assuming a continuous increase of deep electron traps in the EML layer in combination with triplet-polaron quenching (TPQ). The latter also reproduces the characteristic efficiency roll-off observed in the fresh device

## Numerical Analysis of Trap-Induced Negative Capacitance in OLED

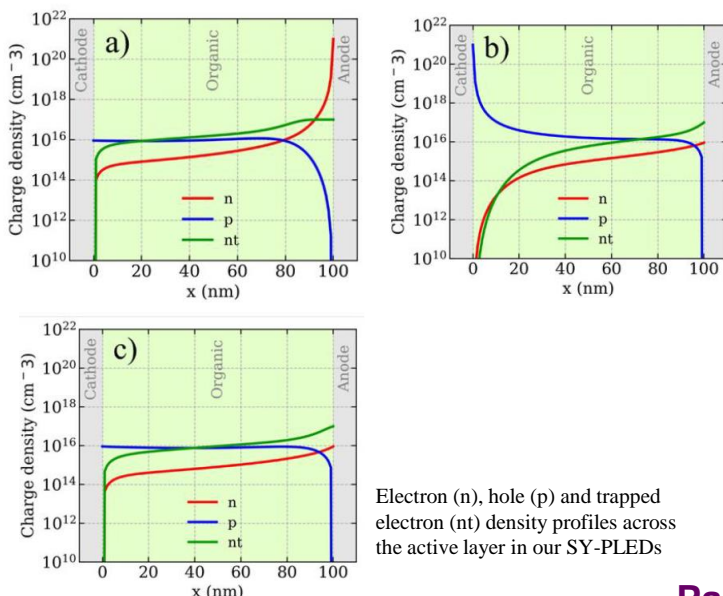
Numerical Analysis of Trap-Induced Negative Capacitance in Organic Light-Emitting Diodes

V. Georgakopoulos-Paltidis\*\*\*, E. Stanzani\*, S. Jenatsch\*, D. Braga\*, B. Blülle\*, B. Ruhstaller\*,\*\*\*

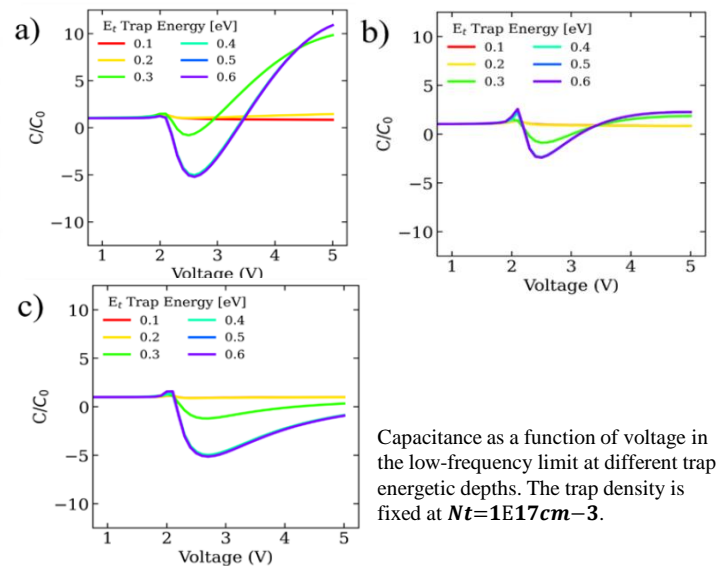
\*Fluxim AG, Winterthur, Switzerland

\*\*University of Bayreuth, School of Mathematics and Natural Sciences, Bayreuth, Bavaria, Germany

\*\*\*Zürich University of Applied Sciences, Institute of Computational Physics, Winterthur, Switzerland

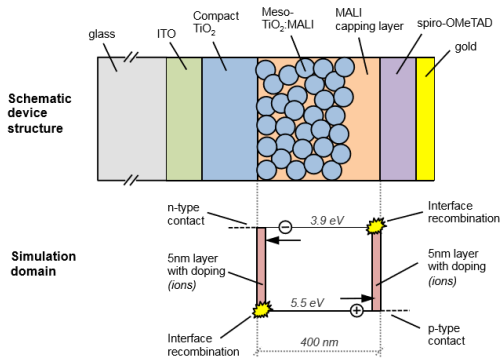


Electron (n), hole (p) and trapped electron (nt) density profiles across the active layer in our SY-PLEDs

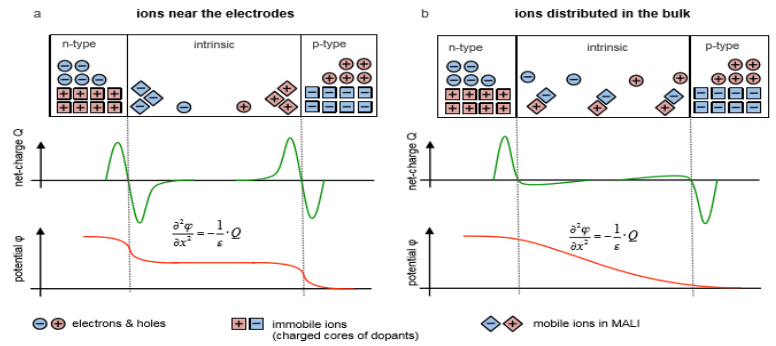


Capacitance as a function of voltage in the low-frequency limit at different trap energetic depths. The trap density is fixed at  $Nt=1E17cm^{-3}$ .

# Setfos-Paios Integration 分析钙钛矿离子效应



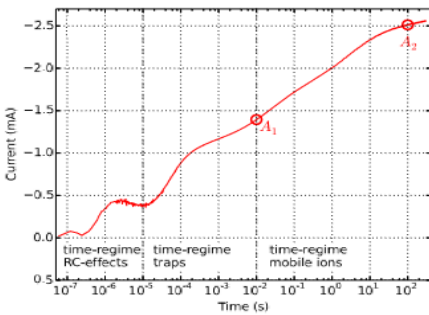
Device structure and simulation domain. The perovskite layer MALI and the mesoporous TiO2 is simulated as one effective medium with one electron and one hole transport level.



Schematic illustration of the effect of mobile ions on the potential. a) Ions are close to the interfaces and screen the electric field inside the bulk. The band is therefore flat. This is the state in the dark. b) Ions are distributed in the bulk and compensate each other. The potential drops over the whole intrinsic region leading to efficient charge extraction.

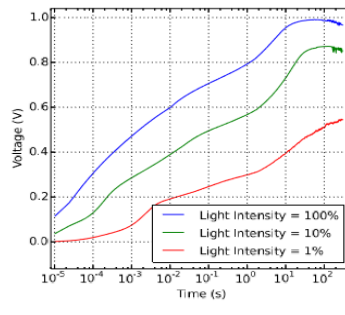
## Paivos Flexible time resolution 8 orders scale

### Transient Photocurrent (TPC)



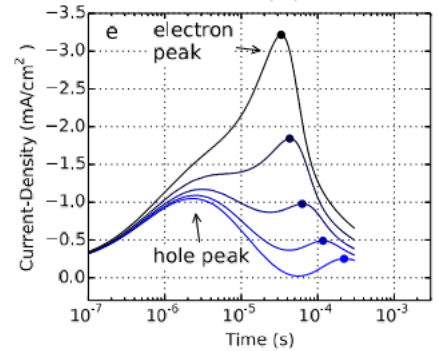
transient photocurrent (TPC) measurement of a perovskite solar cell. A1 and A2 mark two states of the solar cell

### Transient Photo-voltage (TPV)



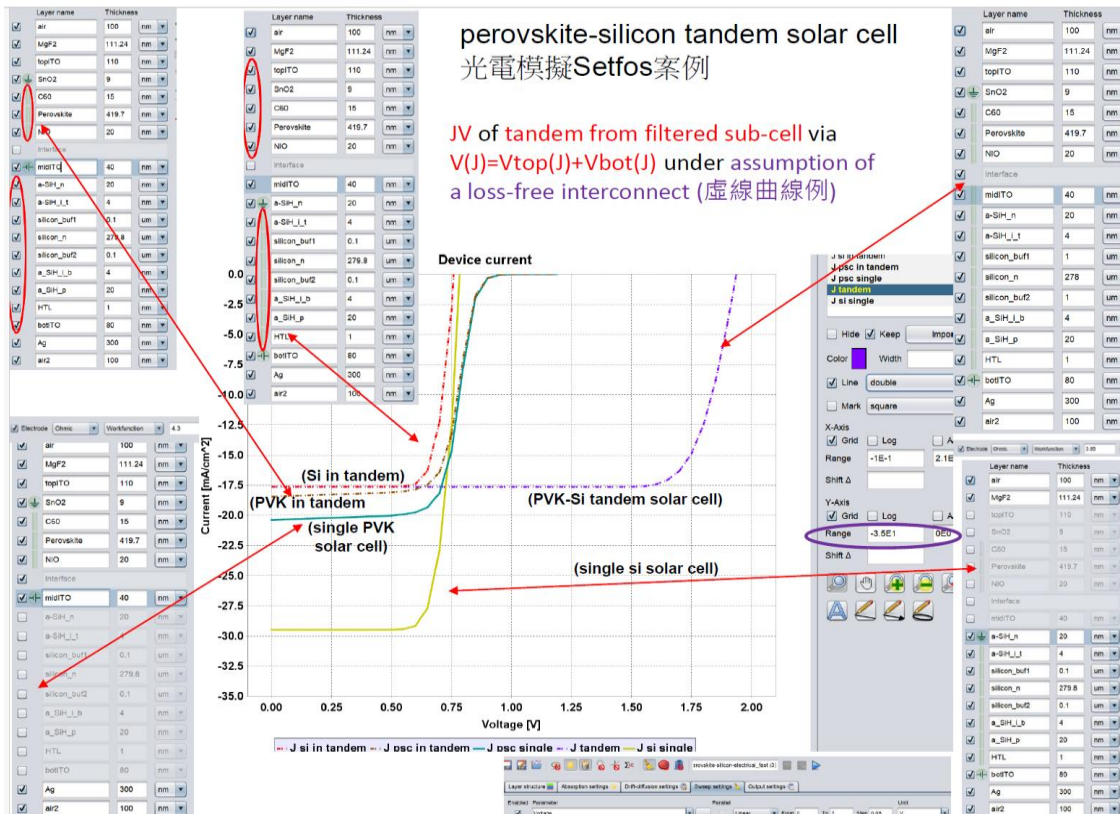
transient photo-voltage (TPV) rise for three different light intensities.

### CELIV



Measured photo-CELIV currents with 5 different ramp rates A in linear

## Pero/Si Tandem Solar Cell Simulation and Optimization



perovskite-silicon tandem solar cell  
光電模擬Setfos案例

JV of tandem from filtered sub-cell via  $V(J) = V_{top}(J) + V_{bot}(J)$  under assumption of a loss-free interconnect (虛線綠線例)

Device current  
(Si in tandem)  
(PVK in tandem)  
(single PVK solar cell)  
(single si solar cell)

# 纳米原子尺度——非平衡条件类费米能级 (Quasi Fermi Level Splitting QFLs) 关键参数, 在实际叠层太阳能电池结构/各个子电池分析辅助以瑞士Fluxim公司Setfos动态仿真模拟

20230117英国Oxford大学, Sheffield大学, 德国Potsdam大学联合paper: Open-circuit and short-circuit loss management in wide-gap perovskite p-i-n solar cells

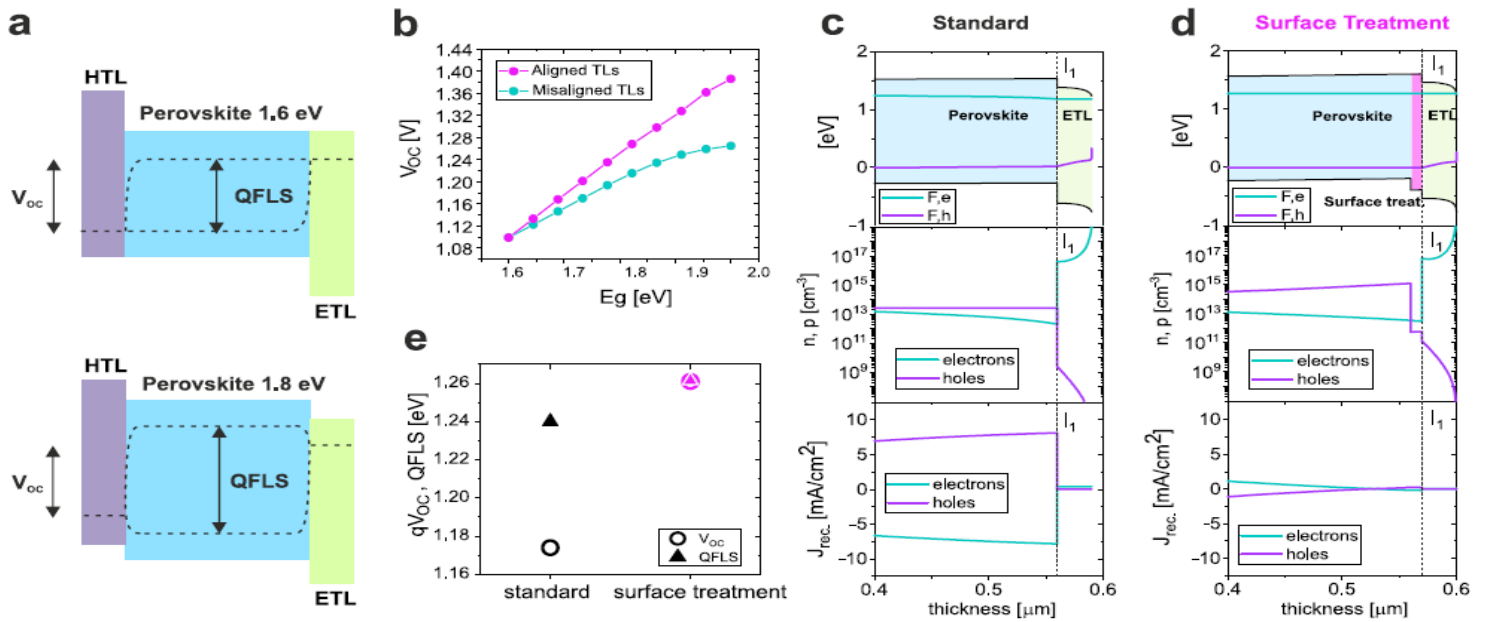


Fig. 1 | Drift-diffusion simulations with SETFOS.

20230504 德国HZB, Potsdam大学等联合paper: Interface engineering for high-performance, triple-halide perovskite-silicon tandem solar cells 32.5%

20230505瑞士洛桑联邦理工学院EPFL, 瑞士CSEM, 澳大利亚昆士兰大学等联合paper: Interface passivation for 31.25%-efficient perovskite/silicon tandem solar cells

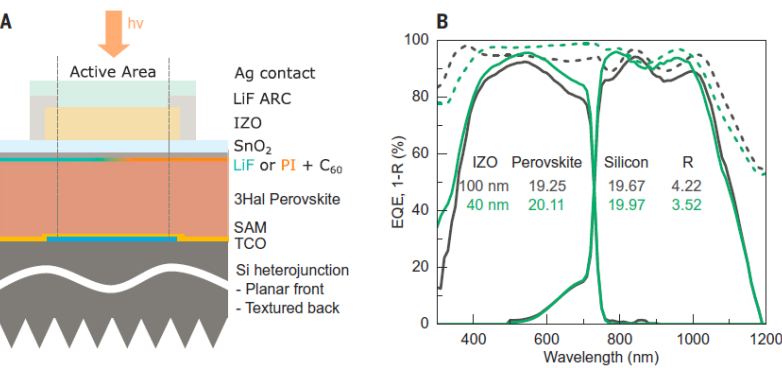


Table S1. PLQY and QFLS obtained from PL measurements on three different device configurations.

Sample	PLQY (QFLS)		
	No surface treatm.	Surface treatment	
	Reference	LiF	PI
Quartz/Perovskite	3.75e-2 (1.305 eV)	9.94e-2 (1.330 eV)	3.93e-2 (1.306 eV)
Glass/ITO/2PACz/3Hal/Surf. Treatm.	5.43e-3 (1.255 eV)	2.47e-2 (1.294 eV)	4.59e-3 (1.251 eV)
Glass/ITO/2PACz/3Hal/Surf. Treatm./C60	2.66e-4 (1.177 eV)	2.34e-3 (1.233 eV)	8.04e-3 (1.265 eV)
Glass/ITO/Me4PACz/3Hal/Surf. Treatm.	4.10e-2 (1.308 eV)	-	2.75e-2 (1.270 eV)
Glass/ITO/Me4PACz/3Hal/Surf. Treatm./C60	2.43e-3 (1.175 eV)	-	9.79e-3 (1.297 eV)

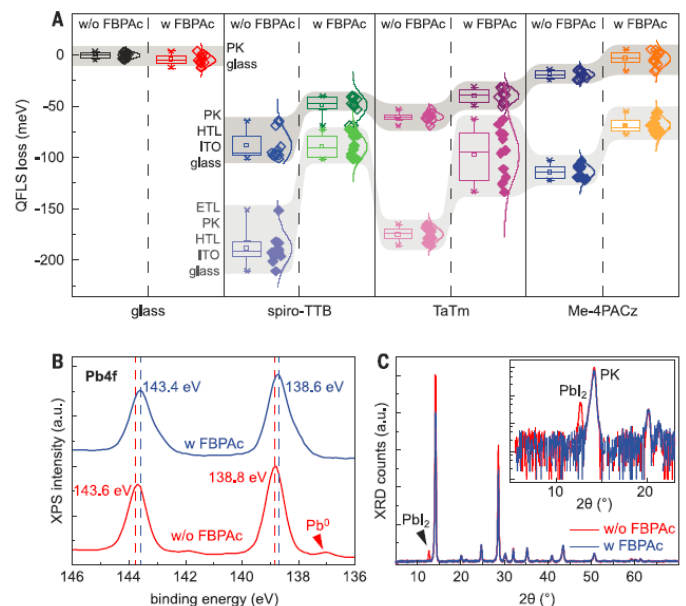
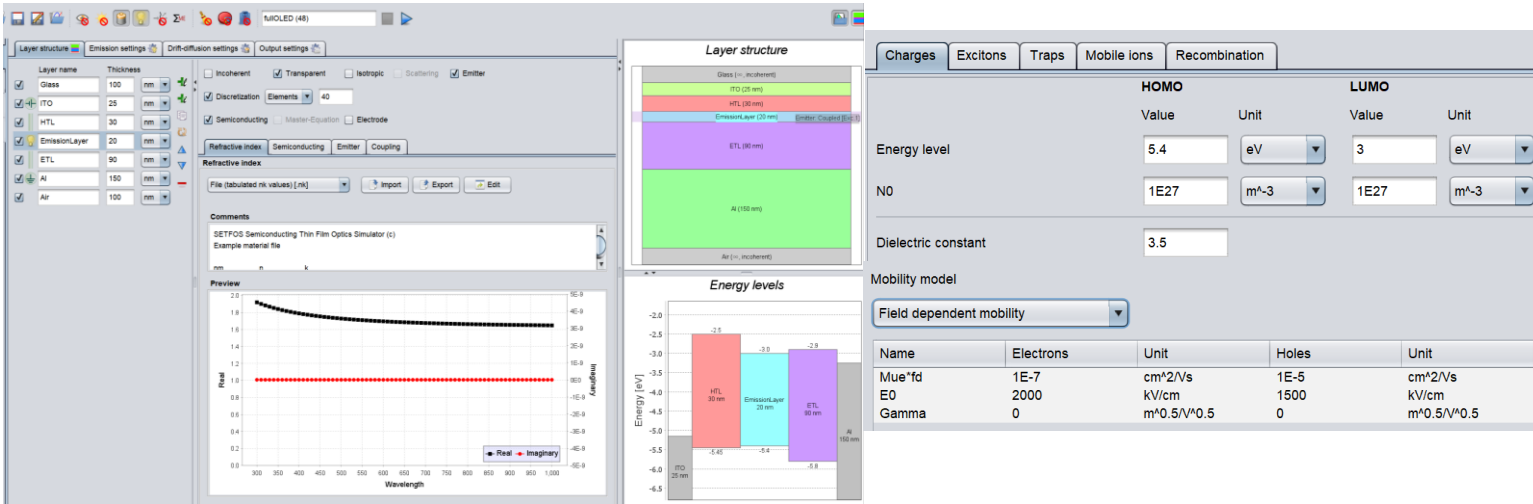


Fig. 1. Reduced nonradiative recombination losses and improved crystallographic properties when adding FBPAc.

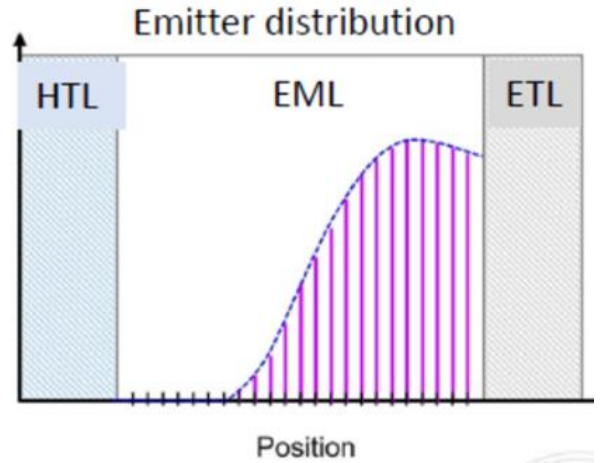
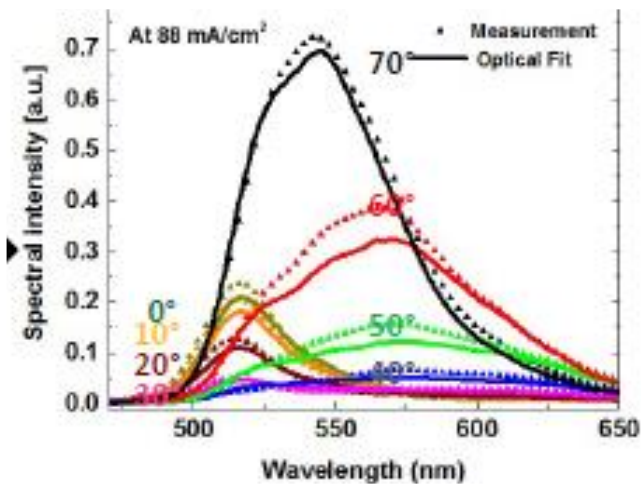


# Setfos

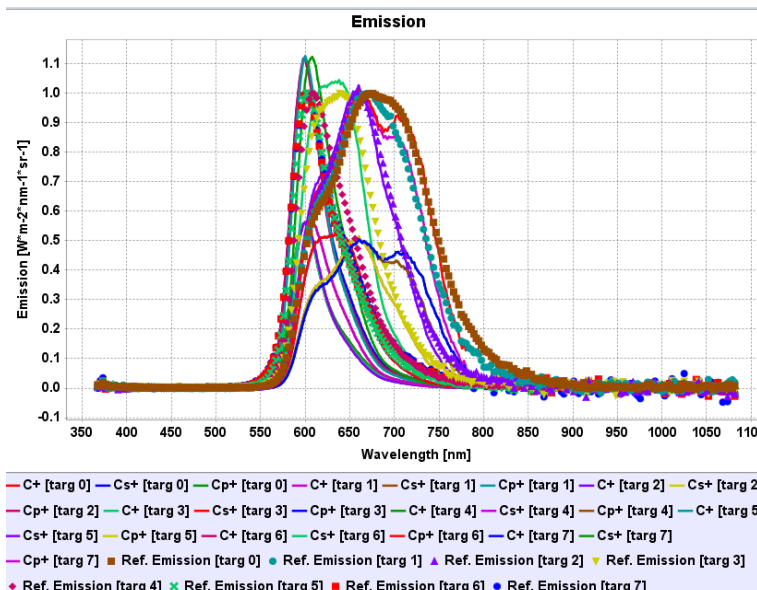
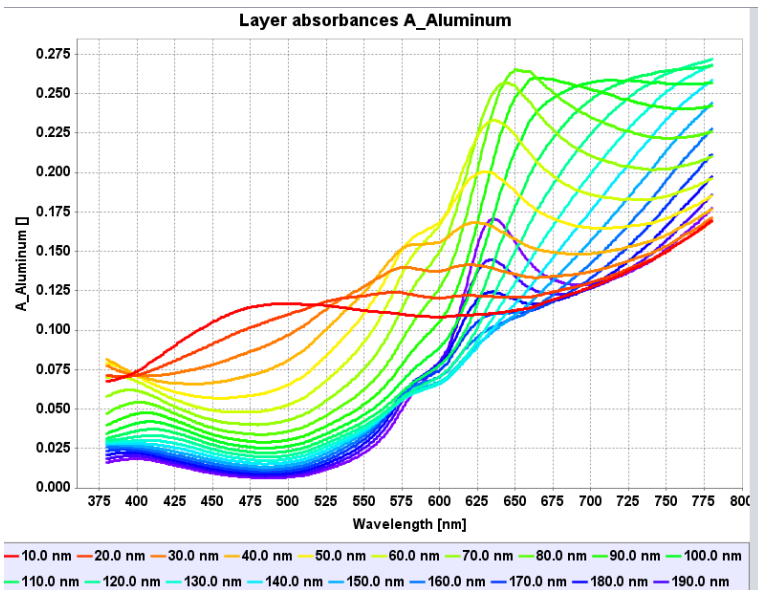
[Setfos设定器件结构参数模拟电性出光结果, 可无限材料器件配置实验]



[可由出光光谱优化或拟合发光层极子(dipole)分布]

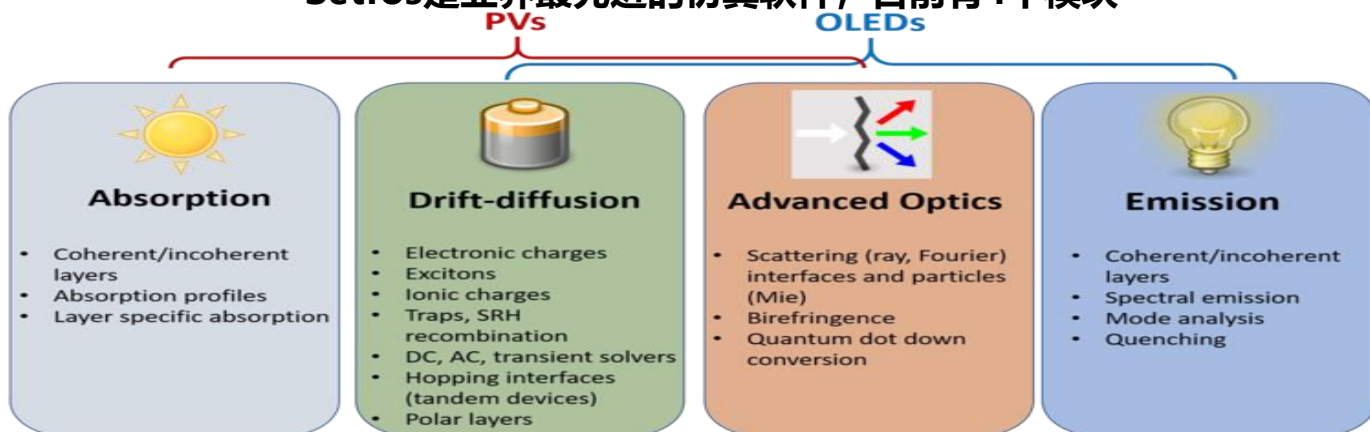


[能扫描参数仿真对应变化趋势, 与对应目标优化参数, 避免繁杂昂贵的反复试验]

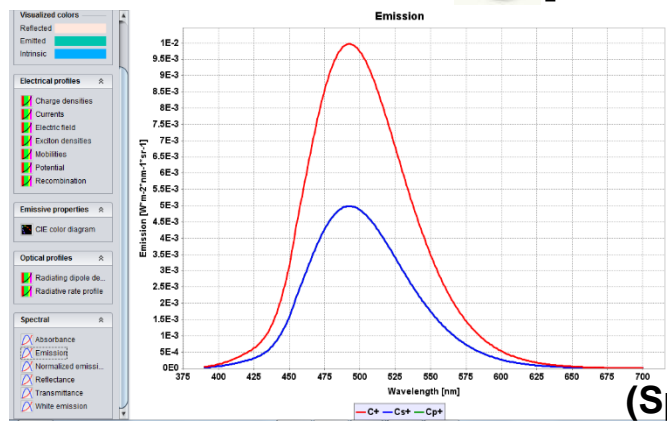


# Setfos

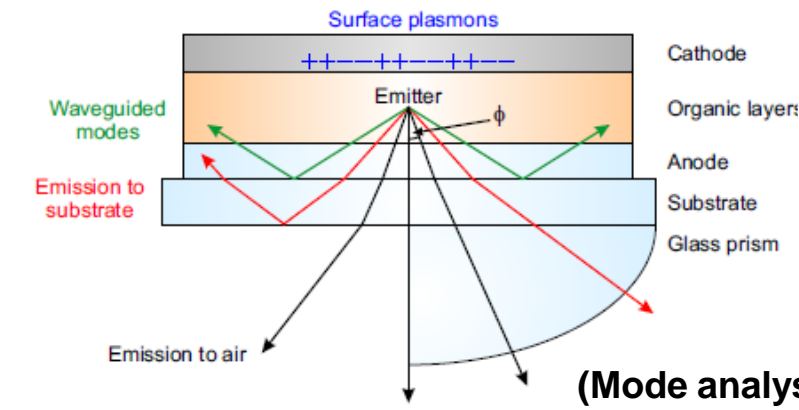
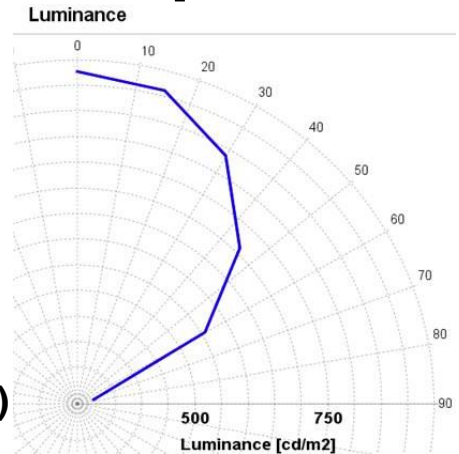
Setfos是业界最先进的仿真软件，目前有4个模块



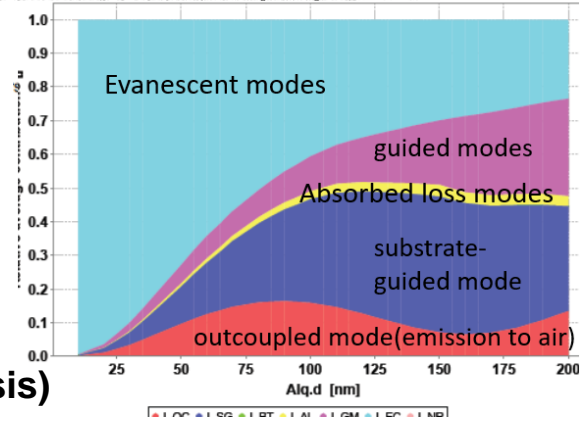
[Emission module]:



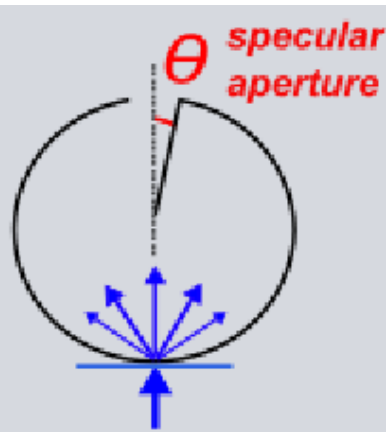
(Spectral)



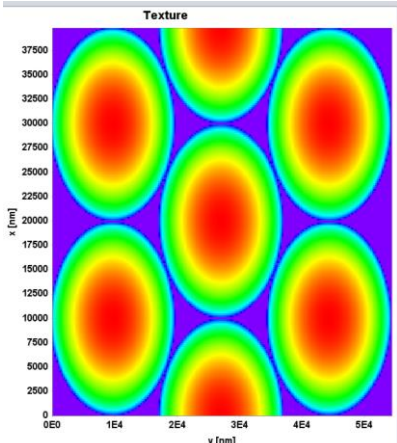
(Mode analysis)



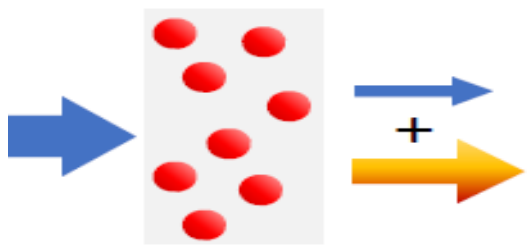
[Advanced Optics module]:



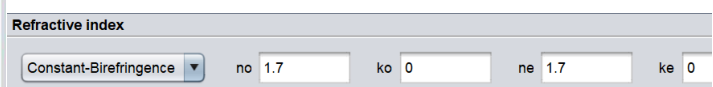
(Haze)



(Microlens)



(QD down-conversion film)



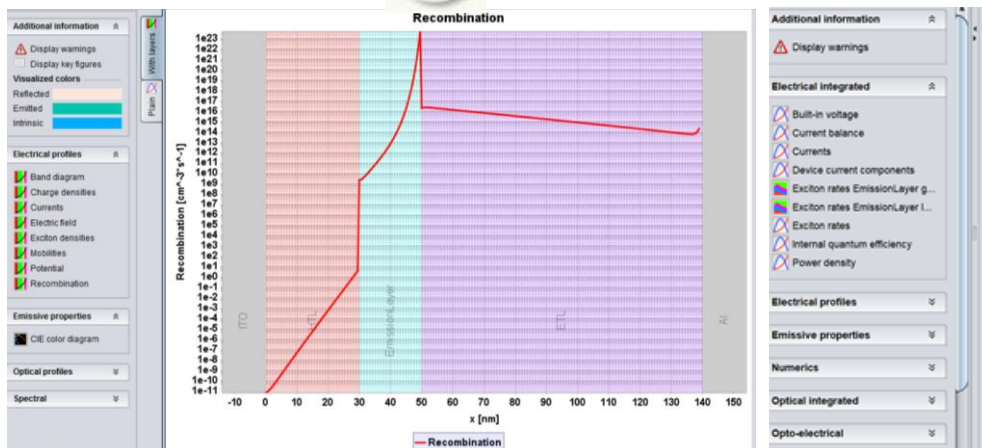
(Birefringence)



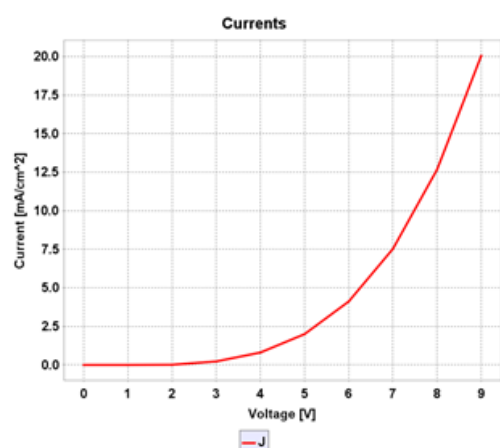
# Setfos



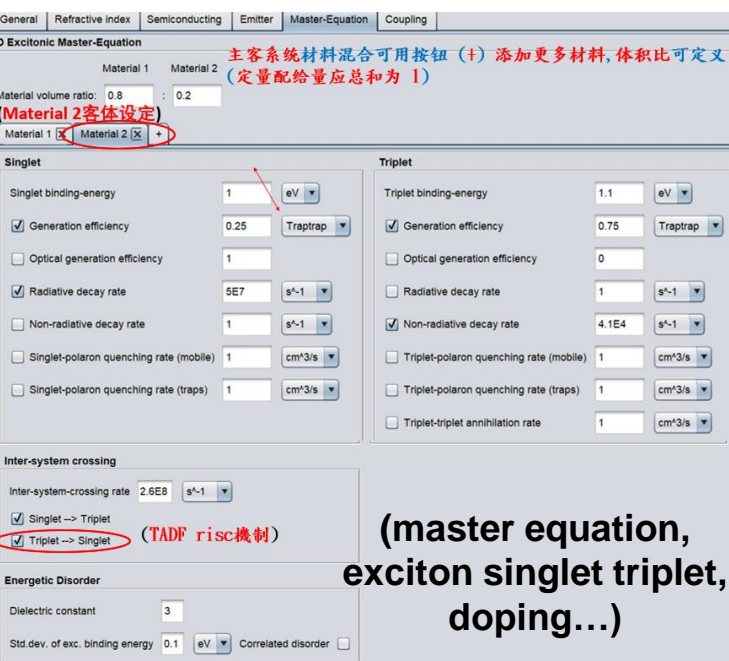
[Drift-Diffusion module]:



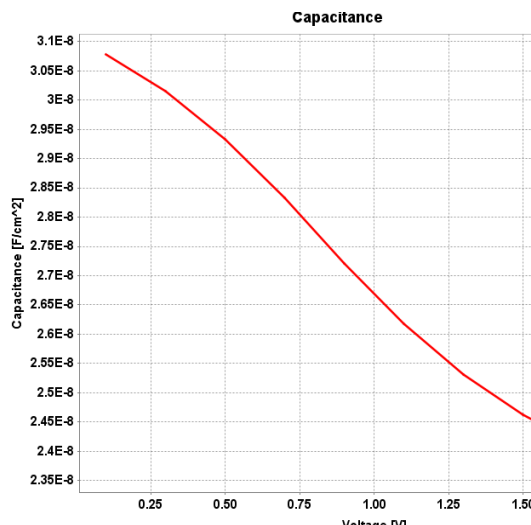
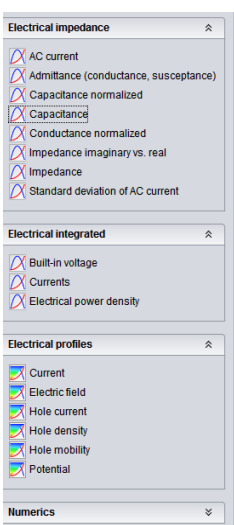
(electrical profile(distribution))



(current voltage)



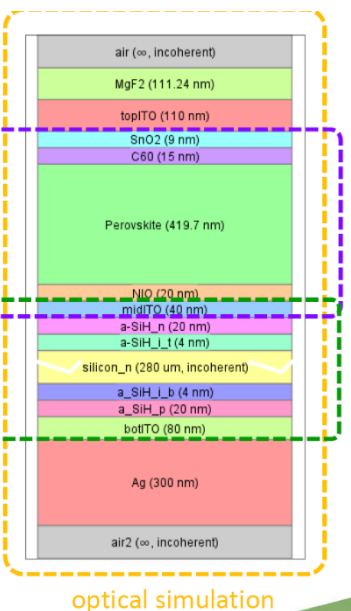
(master equation, exciton singlet triplet, doping...)



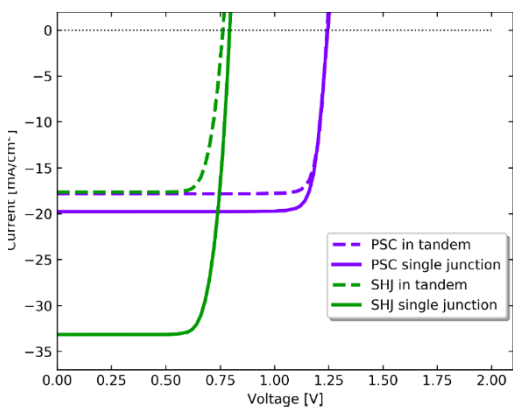
(AC(impedance))



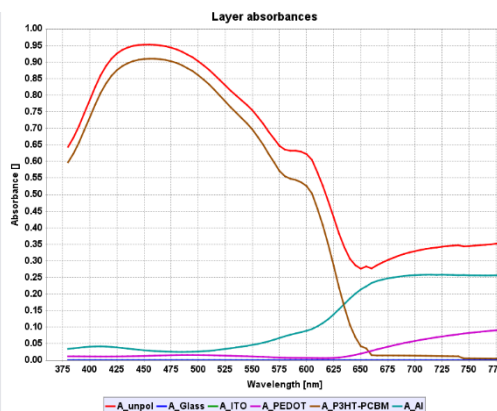
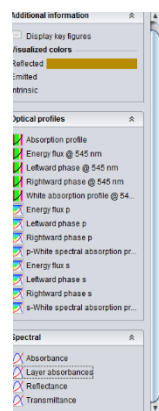
Absorption module:



optical simulation



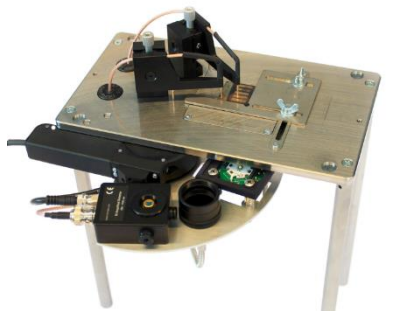
(perovskite-silicon tandem solar cell example)



(Layer absorbances)

# Paios

## Paios 自动量测台及各项功能

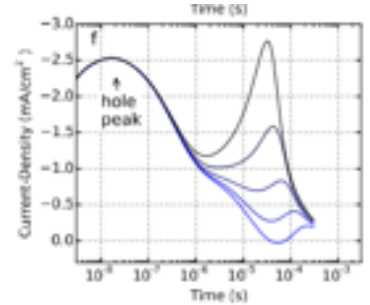
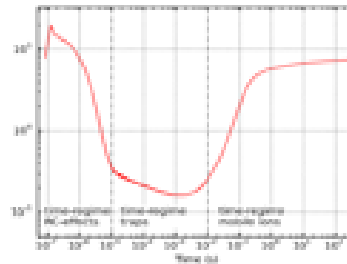
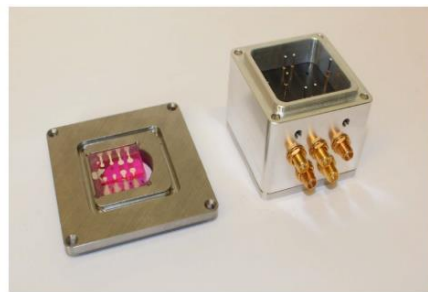


Paios自动测量台：  
可以根据测试项目自  
动旋转



Paios强大的数据后处  
理拟合功能：

- Charge Carrier Mobility from CELIV
- Doping Density from CELIV
- Transport-Time from IMPS
- Lifetime from IMVS
- Series Resistance and Permittivity from Voltage-Pulse
- One-Diode Model Fit
- ions mobility with 8 orders Flexible Time
- Photo-CELIEV for Ions dynamics



Litos: 多通道LEDs/ PV  
ISOS 稳定性测量系统 (支  
持与paios联立使用)

Litos is an advanced LED stability lifetime measurement system. It has 16, or 32 parallel stressing channels distributed over 4 weathering chambers. Each chamber has an individual temperature and illumination control.

### Advantages

- Design customized to customer's sample layout (multiple layouts possible)
- Modular: connect several systems together
- Compatible with external atmosphere-controlling equipment
- Automatic parameter extraction and plotting over time

### Technical Specification

Voltage range	-9 V to 9 V
Maximum current	60 mA /channel
Temperature range	0 - 85 °C
Sample size	Up to 20mm diameter
Illumination	390nm (UV), 450nm + 580nm (white)

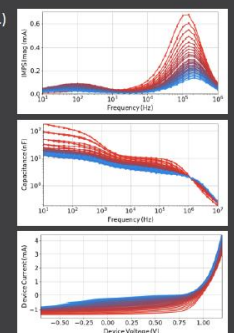
### Litos Features

- Advanced lifetime analysis
- 16 or 32 parallel channels
- Flexible sample design
- Temperature control
- 4 weathering chambers
- Fully automated
- Professional, user-friendly software

LED

When paired with our platform Paios repeated full characterization of the devices can be automatically performed including:

- Transient measurements (CELIV, DLTS, TPV, TPC, TEL...)
- Impedance spectroscopy / CV / IMPS / IMVS
- Dedicated stressing routines for OLEDs
- All measurements as function of temperature

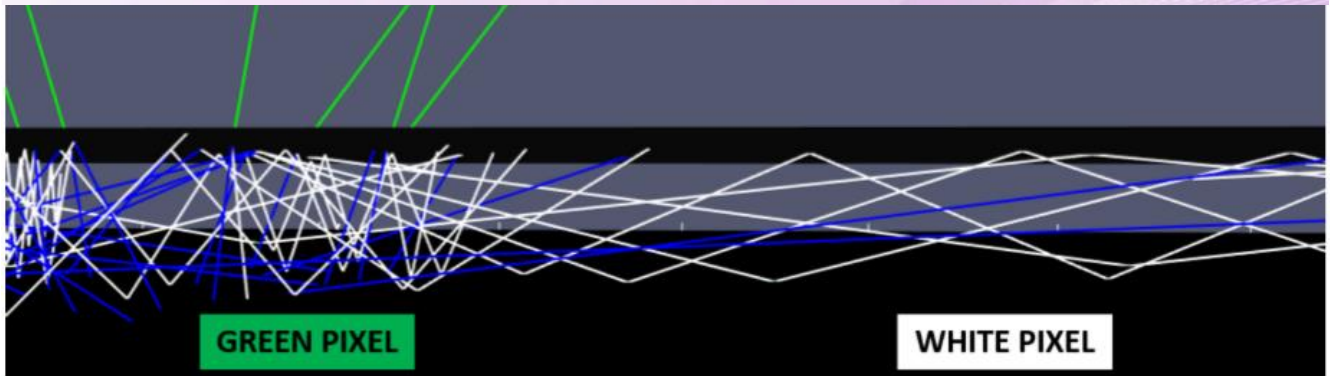




# LAOSS

## 光模块

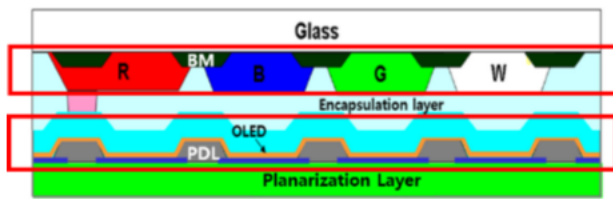
易于使用的光线追踪系统，用于仿真3D光学组件。该模块可以容易地与Setfos [4]结合，以分析具有复杂光耦合几何结构的OLEDs和太阳光电系统



Cross-section view of an WOLED/CF display. Blue rays are assigned as primary rays, which are emitted from the white OLED. White rays are reflected/transmitted rays and green ones are the rays reaching the detector.

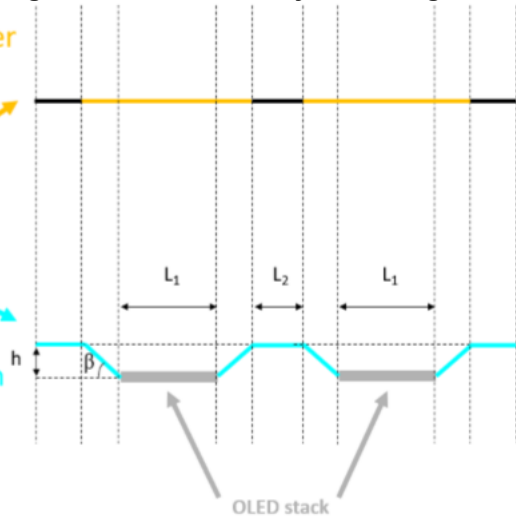
## 光串扰crosstalk解决方案

Color Filter Interface

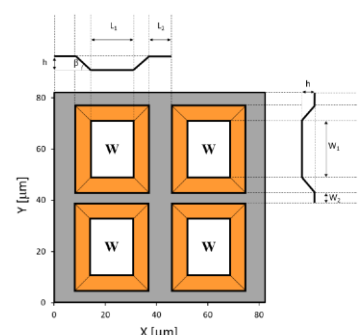
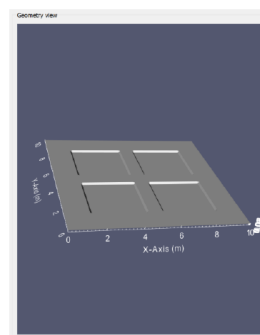
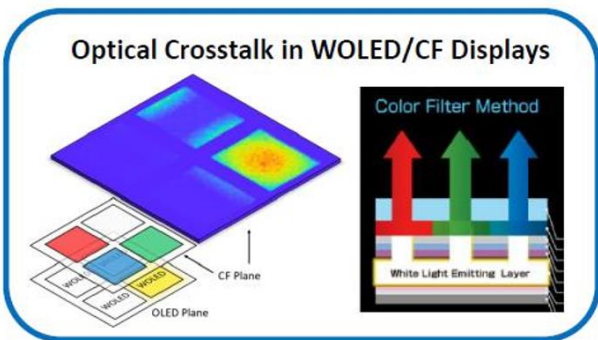


Geometry of the OLED layer.

Pixel Definition Interface



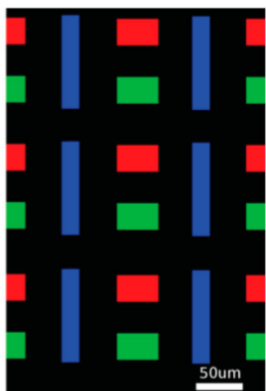
## 模拟OLED显示器中的光学串扰



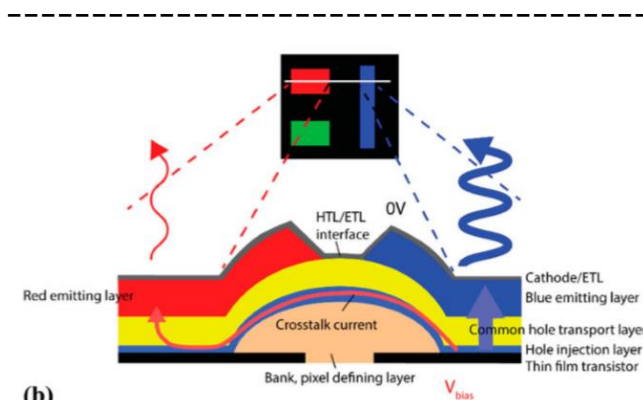
在测试白光OLED / 色彩滤波矩阵中透过未开启单位的滤色器 (CF) 漏光

## 电模块

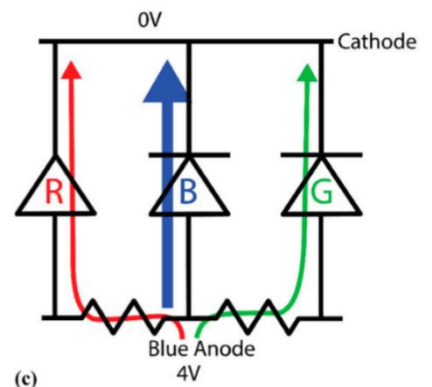
## 电串扰crosstalk解决方案!



(a) swiss made



(b)



(c)



# Phelos

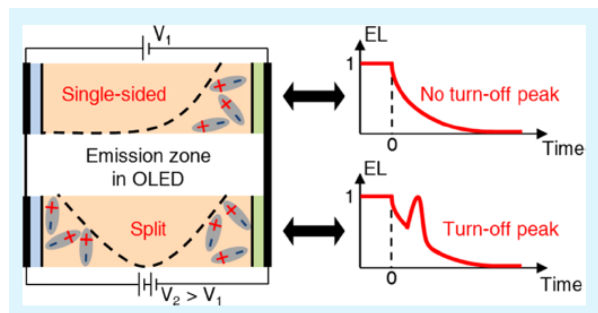
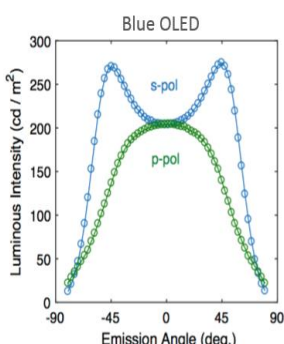
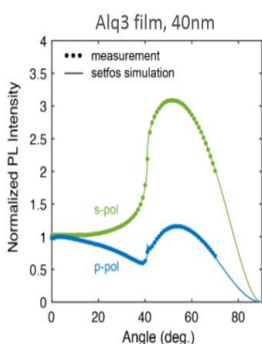
**phelos**  
angular luminescence spectrometer

- OLED efficiency
- Viewing angle
- Emitter orientation and position
- One-click operation

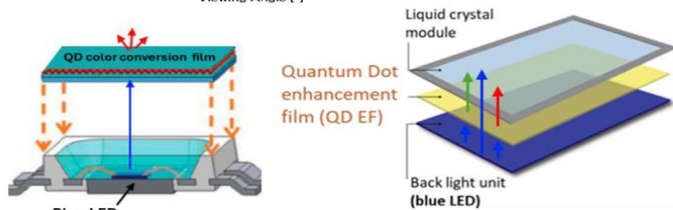
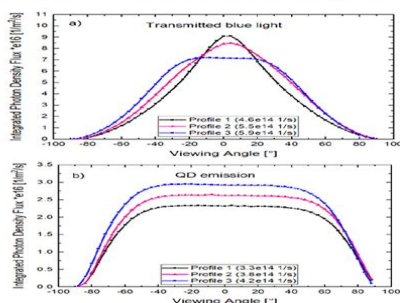


**Phelos**是针对OLED器件的发光特性量测而设计的，它可以量测再不同角度不同偏振下的器件的EL和有机材料PL光谱，再通过计算或者与Setfos模拟软件搭配获得OLED器件或者有机材料的其他参数，例如：IVL, EQE, lm/W, Cd/A, CIE<sub>x,y</sub>, 以及发光层材料分子取向，以及分子分布情况等。

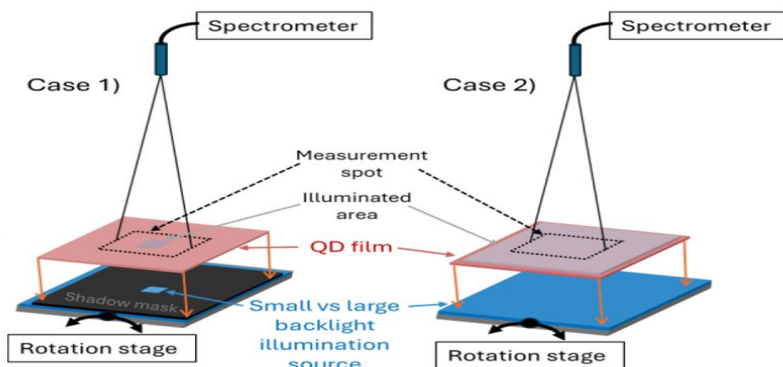
光致发光和电致发光:发射器内分子的偶极方向和位置



## Modeling the Impact of the Illumination Geometry on the Light Conversion Efficiency in Quantum Dot Down-Conversion Films



$$LCE = \frac{\int^{color} I_{QD}(\lambda) d\lambda}{\int^{blue} I_{BLU}^{illuminated}(\lambda) d\lambda - \int^{blue} I_{BLU}^{transmitted}(\lambda) d\lambda}$$



除了 QD 膜的厚度和浓度，我们利用 Phelos 和 Setfos 的整合运用深入分析并且提取入射背景光源的几何形状(Geometry)和入射角(Angular)对 LCE (Light Conversion Efficiency)的影响，更提高 QD 膜使用效果！