Bridging the Scales:

Towards Parameter-Free Simulation-Aided OLED Design from Molecule to Device

Outline

- Introduction to Simbeyond
- Bumblebee: 3D kinetic Monte Carlo tool for OLEDs
- Simbeyond & SCM, towards a parameter-free multiscale toolchain from molecule to device
- Application of multiscale toolchain to TADF and hyperfluorescent materials and devices (Case studies with Cynora)

Simbeyond: accelerating OLED R&D

Commitment:
Reduce time to market and improve performance of OLED materials and applications by providing **predictive 3D simulation tools**

Markets:
OLEDs for displays, signage, and lighting; OPV; OFET

Users:
Chemical suppliers, device manufacturers, technology centers, and universities

Team expertise

What Simbeyond brings to OLED R&D teams

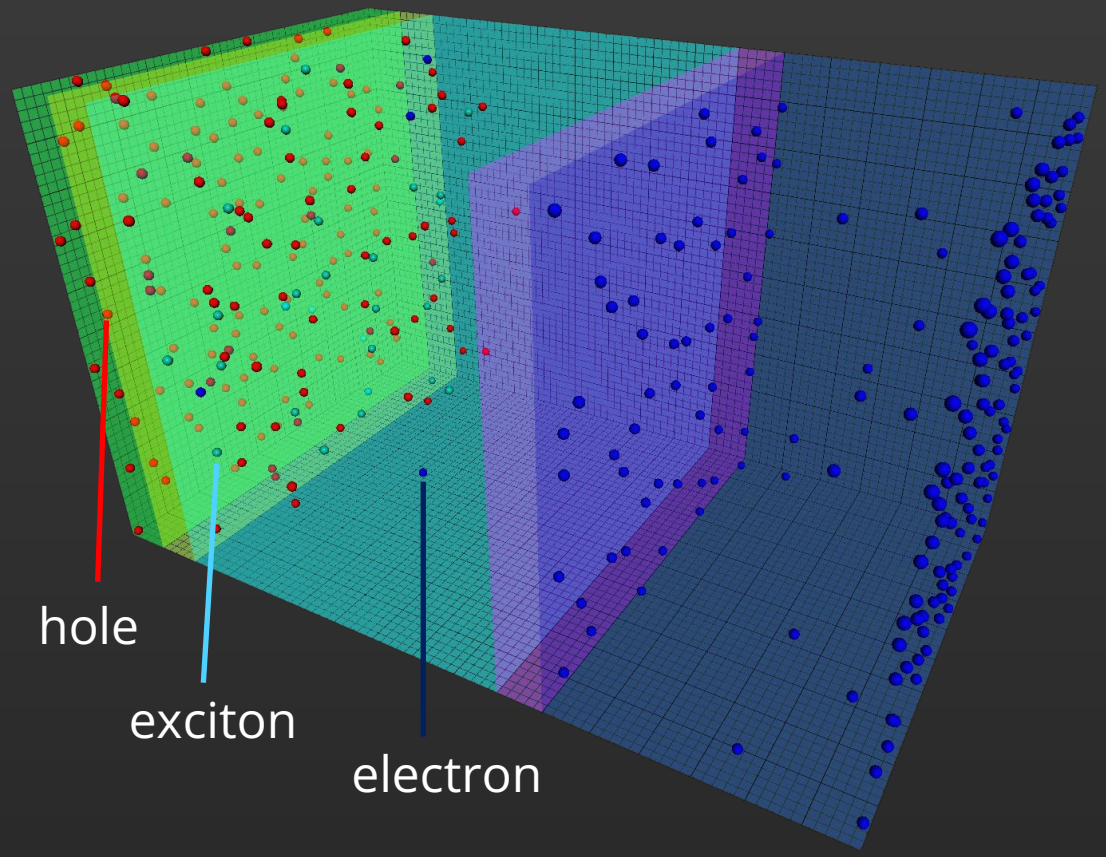
- Simulation software based on former **Philips OLED research and IP**
- Competences - Simbeyond employees have **PhDs in:**
  - OLED Device Physics
  - Materials Science
  - Computational Chemistry
- Advisory board and team includes **worldwide renowned experts** in OLED R&D, scientific modeling and simulation
- Customers include some of the **largest companies active in OLED**
- **Many universities** using Bumblebee

Bumblebee: ultimate OLED device simulator

bumblebee™

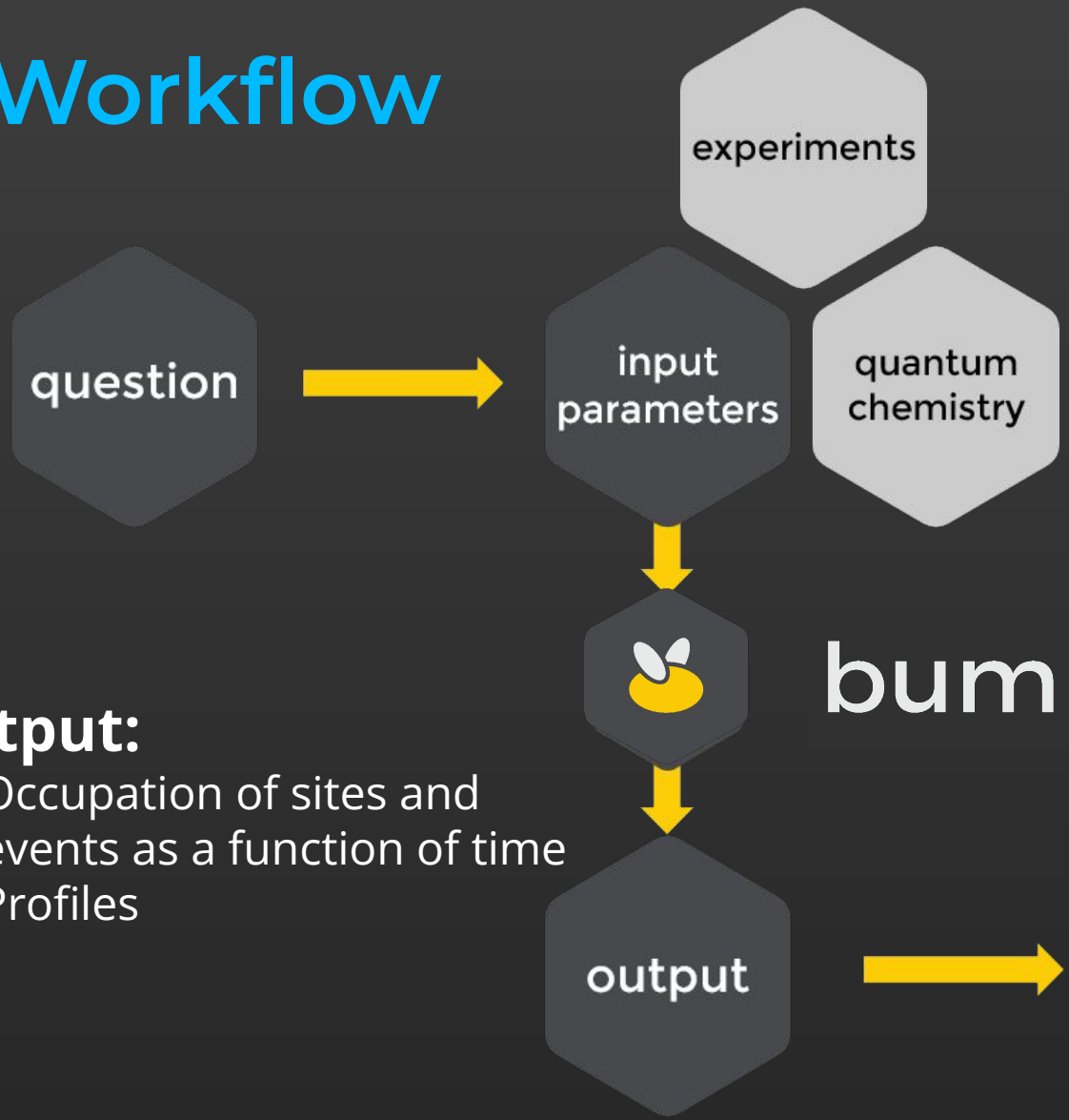
- Predictions of device performance far beyond present tools
  - Electrical characteristics
  - Efficiency (roll-off)
  - Color point and color stability
  - Device degradation scenarios
  - Lifetime prediction

- Time and 3D spatially resolved views of device functioning
- Convergent simulations
- Intuitive user interface



Linking nanoscale material properties to macroscopic device performance

Workflow



Input:

- Materials Parameters
- Stack definition
- Morphology
- External conditions

Post-Processing:

- Current-voltage curve
- Efficiency
- Lifetime

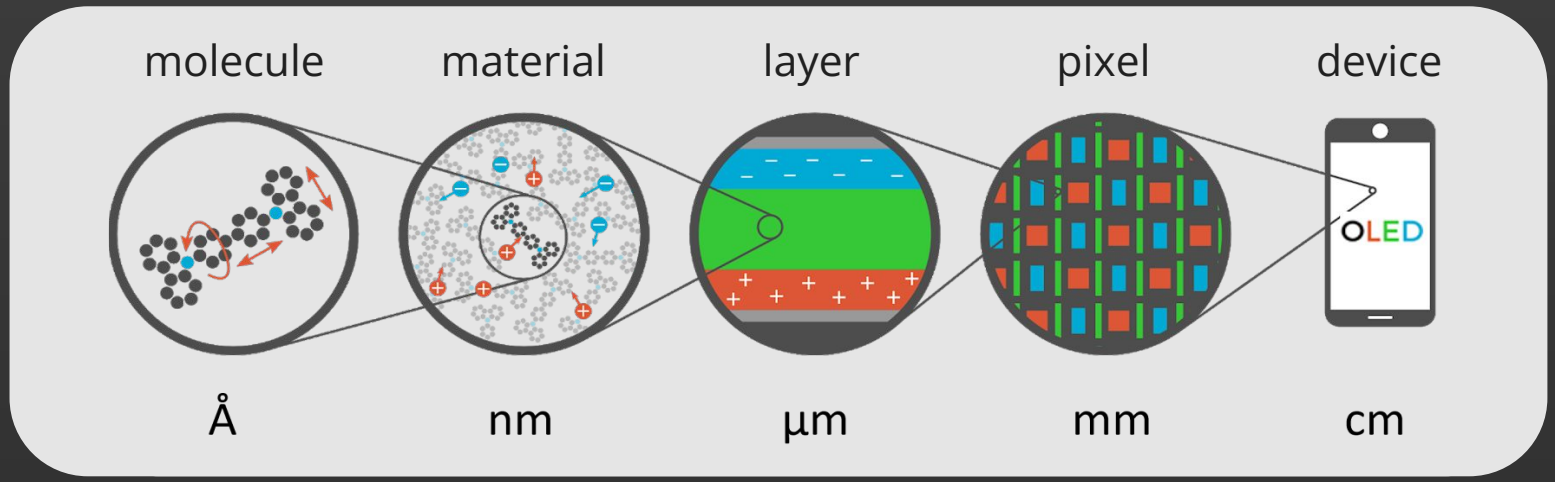
Output:

- Occupation of sites and events as a function of time
- Profiles

Simbeyond & SCM:

Towards a parameter-free multiscale toolchain from molecule to device

Collaboration between Simbeyond & SCM:



Roles of partners in the toolchain

SCM

Calculating molecular level properties such as:

- IP/HOMO and EA/LUMO energies
- Exciton energies
- Transfer integrals

of each molecule in a realistic morphology

SIMBEYOND

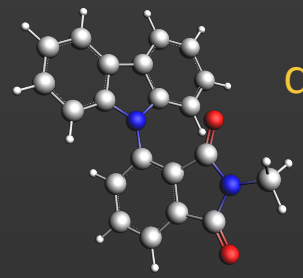
Scaling of molecular level properties to device level and calculating device level properties such as:

- Charge transfer properties - *J*(*V*)
- Excitonic events - EQE
- Loss processes

in real 3D device dimensions

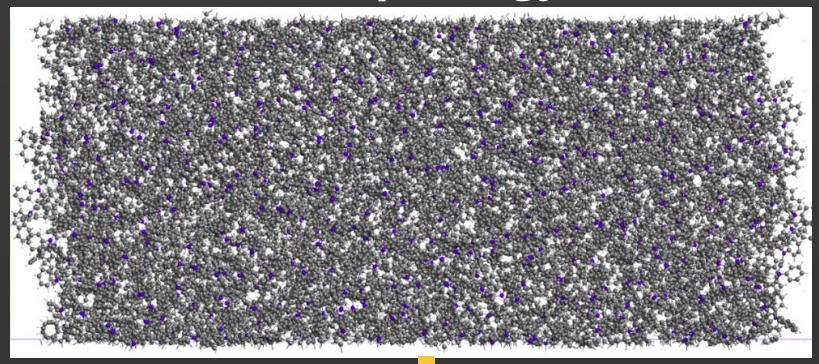
Multiscale toolchain: overall workflow

Molecule



deposition

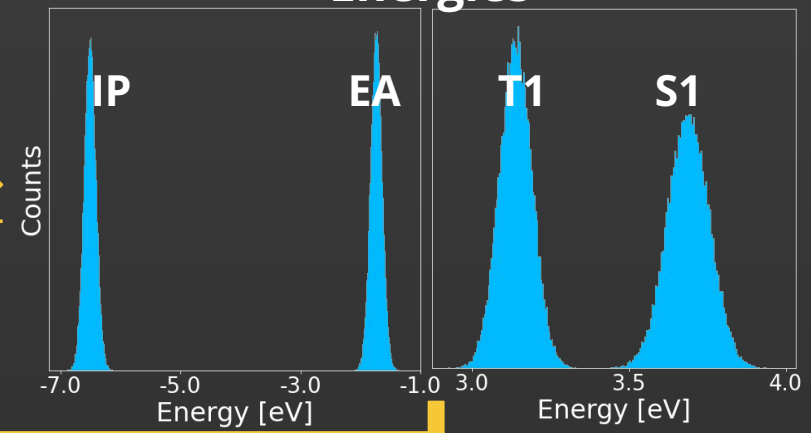
Morphology



DFT

TDDFT

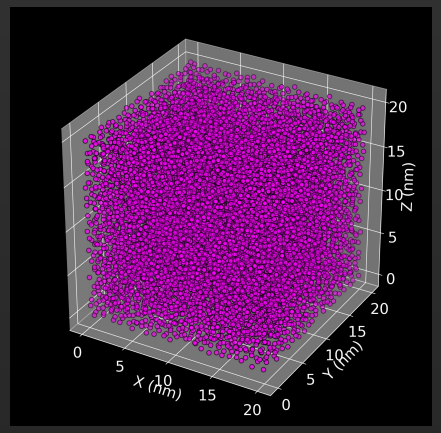
Energies



morphology scaling

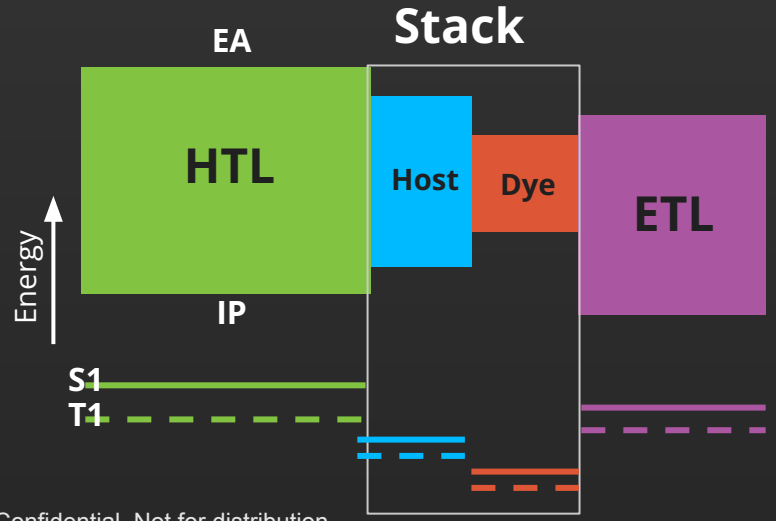
energy scaling

Layer



stacking

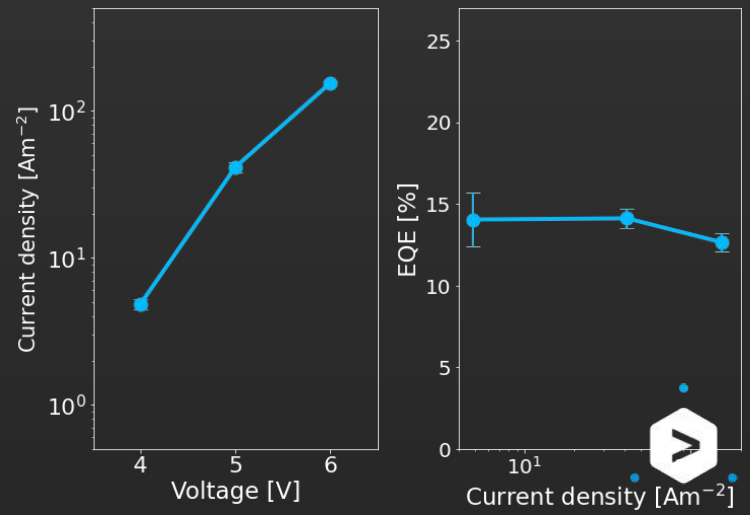
Stack



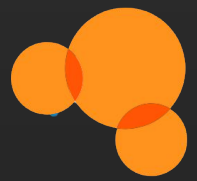
KMC

ME

Device Results



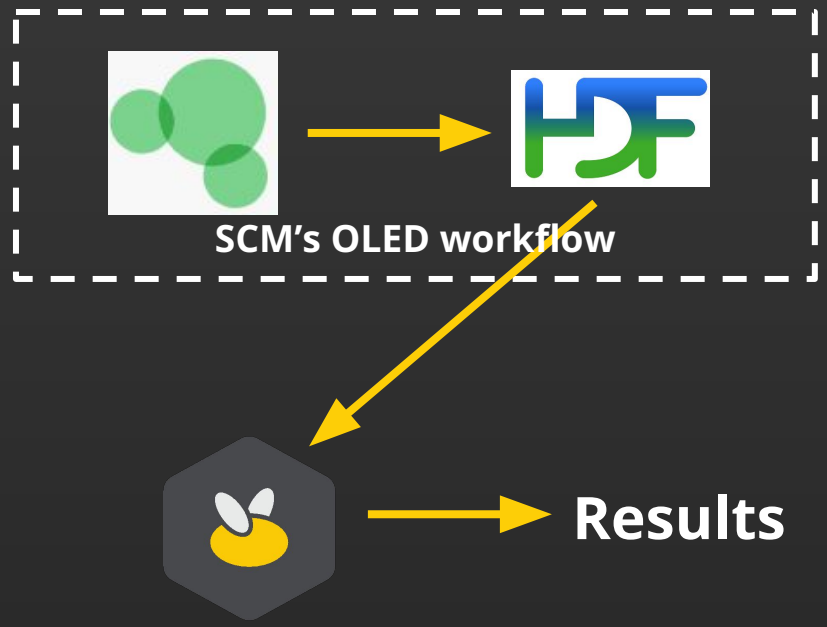
Demo time (SCM)



Connecting AMS and Bumblebee

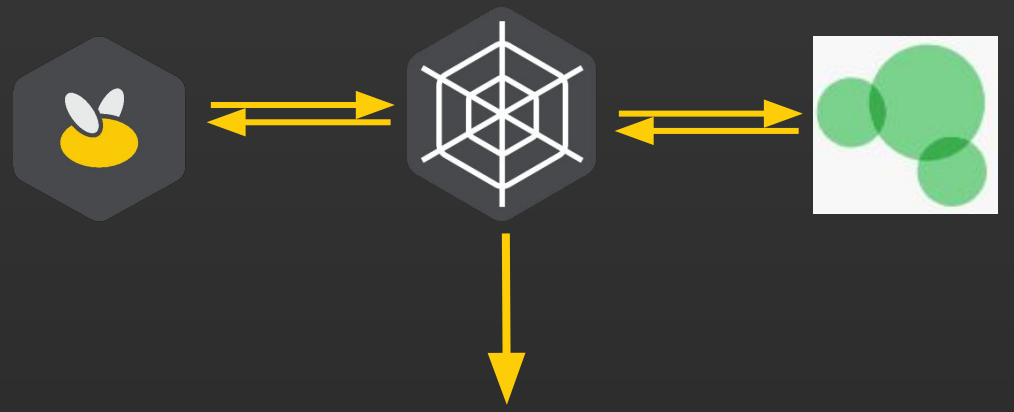
Option 1

Using already generated hdf5 files for the layers of the OLED



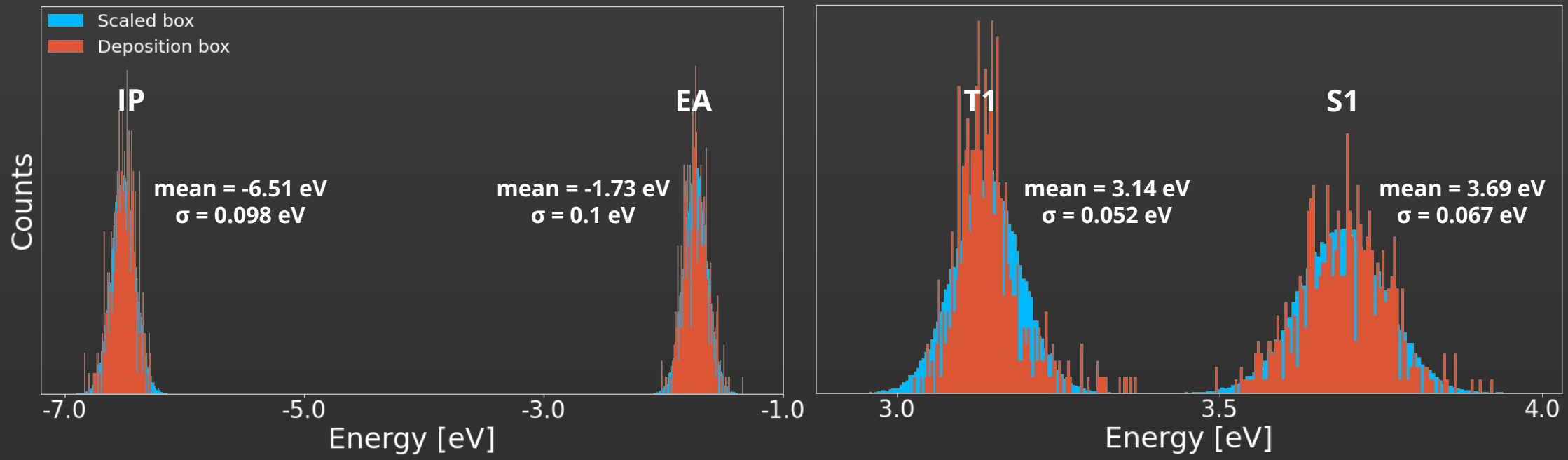
Option 2

Using Simbeyond's Spiderweb environment for the automated workflow



Demo time (Simbeyond)

Energy scaling

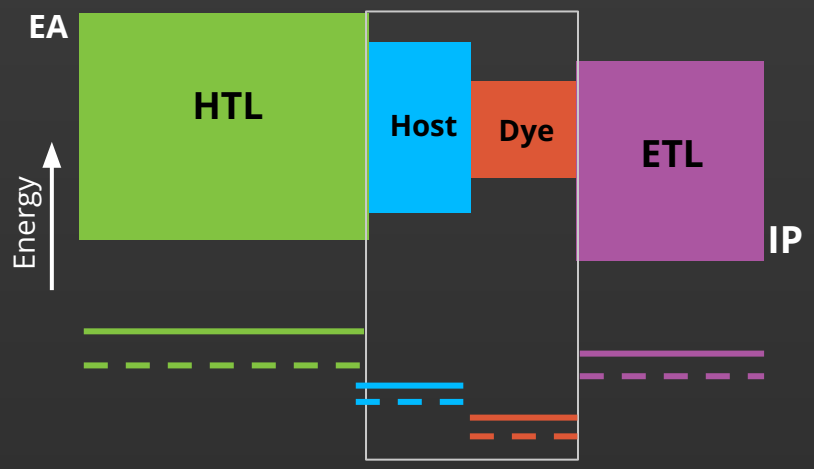


- Each molecule's environment is taken into account with a polarizable QM/MM scheme using DRF method
- IP/EA energies: Delta-SCF method (framework of DFT)
- Exciton energies: TD-DFT with hybrid functionals
- The energies in the deposition boxes are scaled up to the device level, whilst keeping the mean and the sigma of the IP/EA and exciton energies identical

* Baumeier et al. PRB **86**, 184202 (2012)

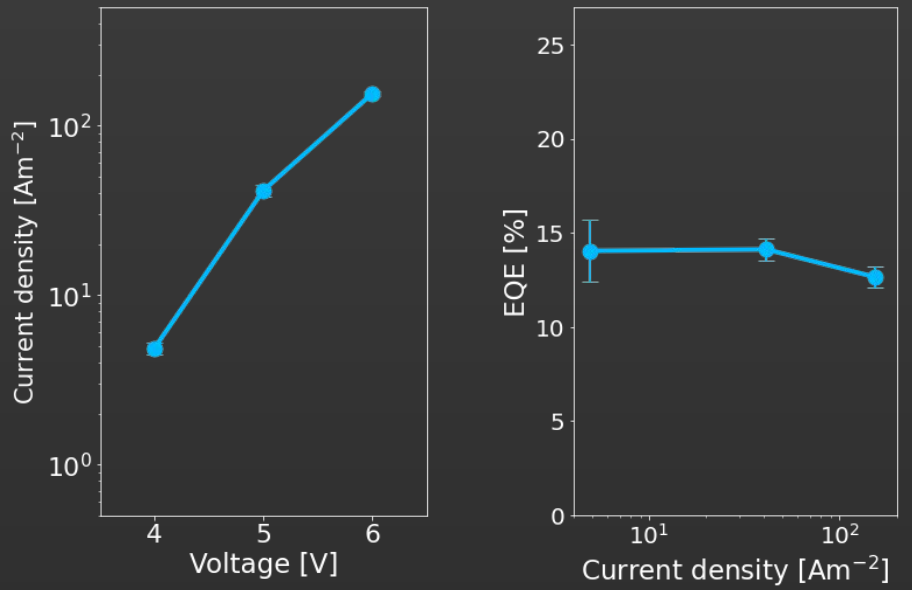
Device level simulations

Stack



Device simulation engines

Device Results



Available device simulation engines:

- 3D kinetic Monte Carlo
- 3D Master equation

Example capabilities of the multiscale toolchain:

- Predictive simulations for charge and excitonic processes
- Trend analysis for the *J*(*V*) and EQE for different devices
- Sensitivity analysis of various parameters

Case study with Cynora

Trend analysis on the *J*(*V*) and EQE of devices based on TADF and hyperfluorescent materials with different host-guest concentrations in the EML

TADF devices

EML concentrations:

- Device 1 = 9.3 mol% T; 90.7 mol% H
- Device 2 = 20.0 mol% T; 80.0 mol% H

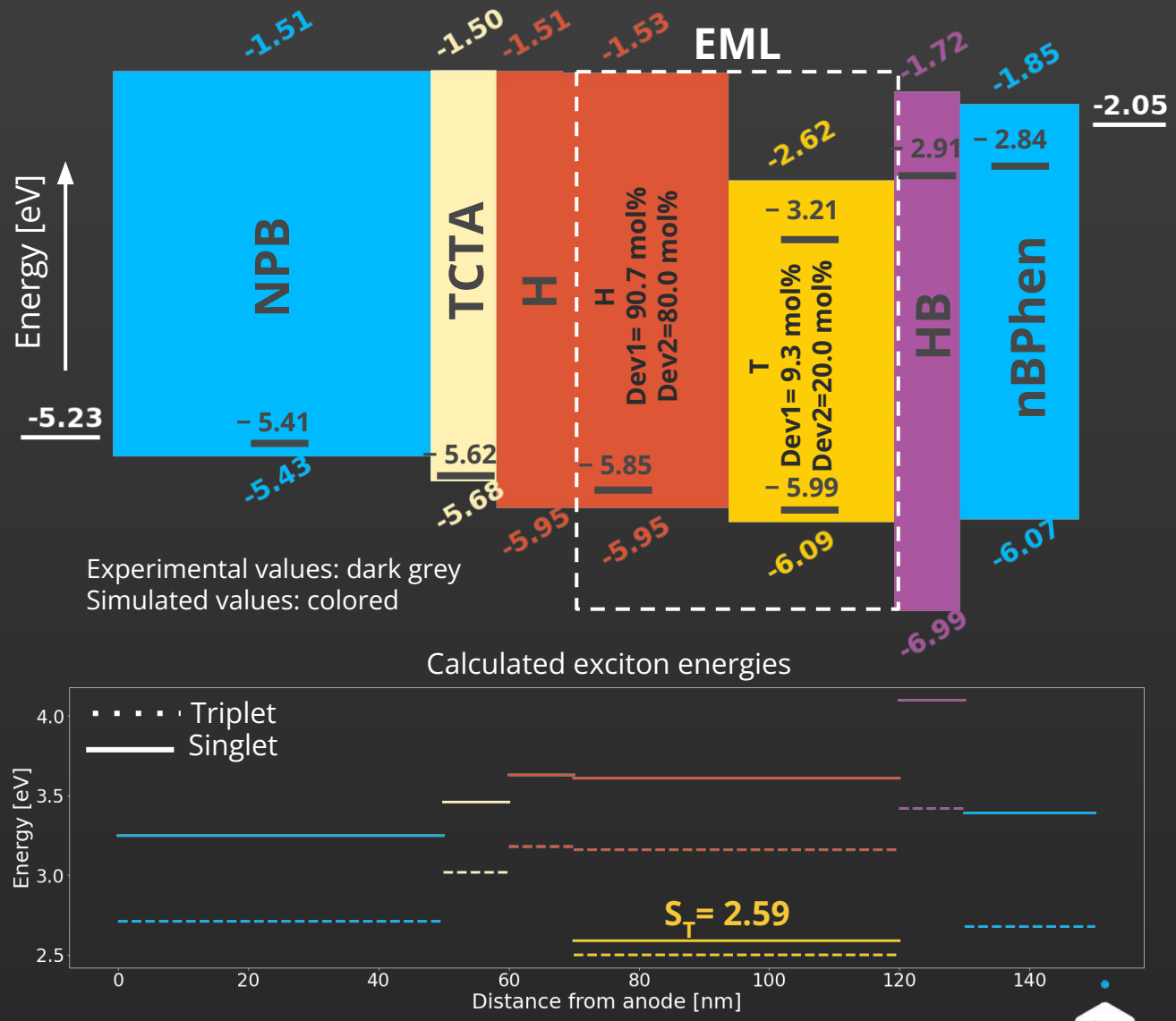
Task of the case study:

Trend analysis on the *J*(*V*) and EQE of TADF devices with different host-guest concentrations

Approach:

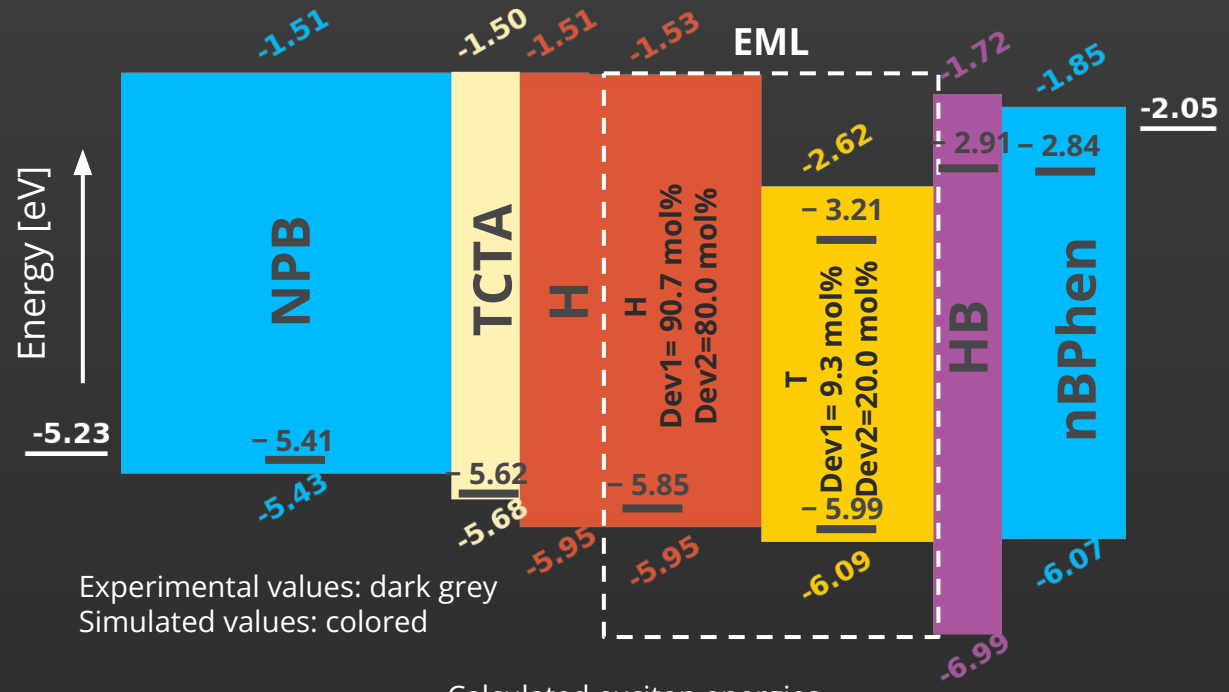
Multiscale toolchain:

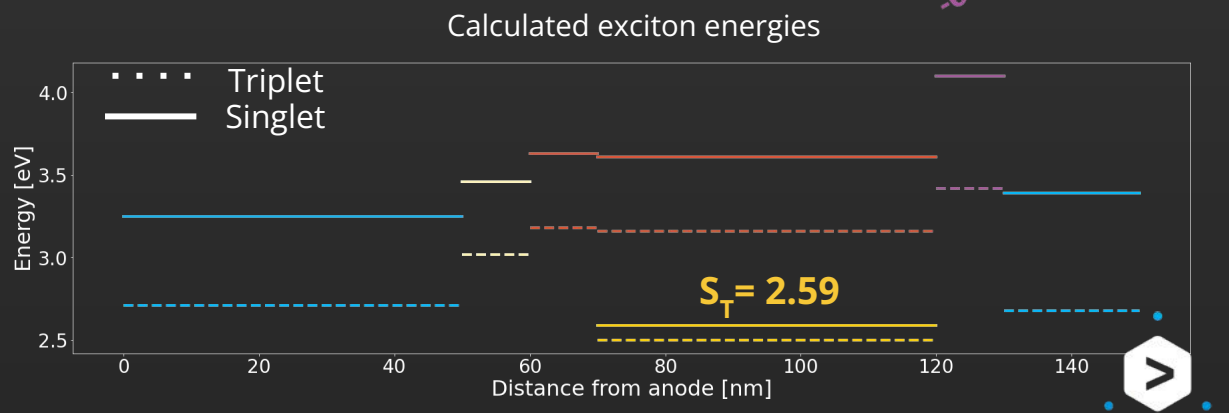
- HOMO, LUMO, and exciton energies
- Up to device performance



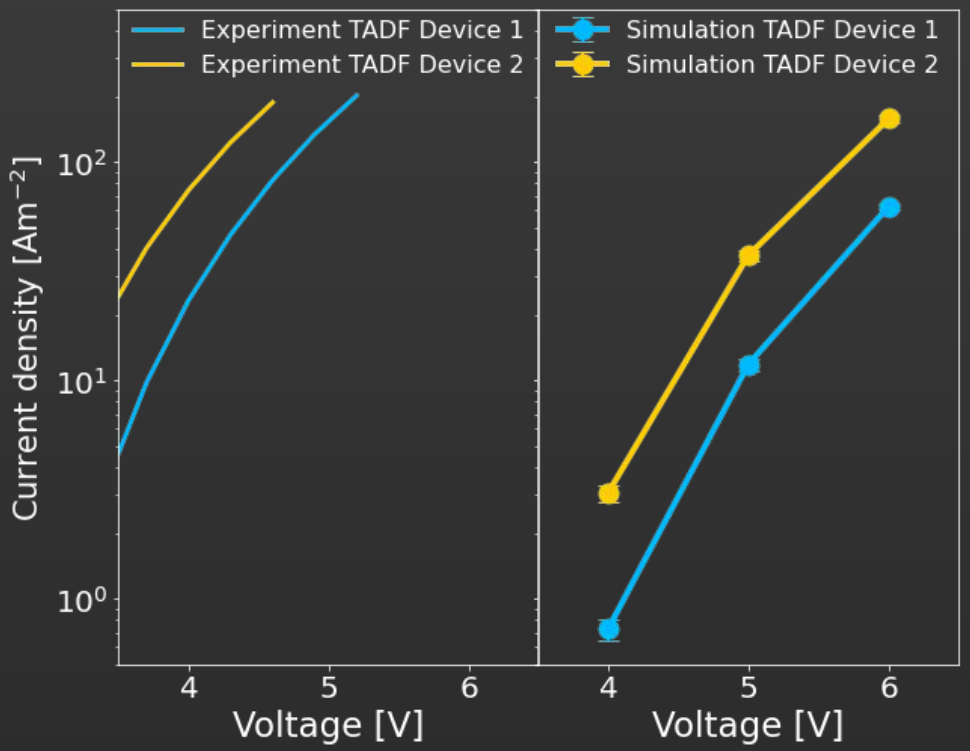
Molecular scale predictions - TADF

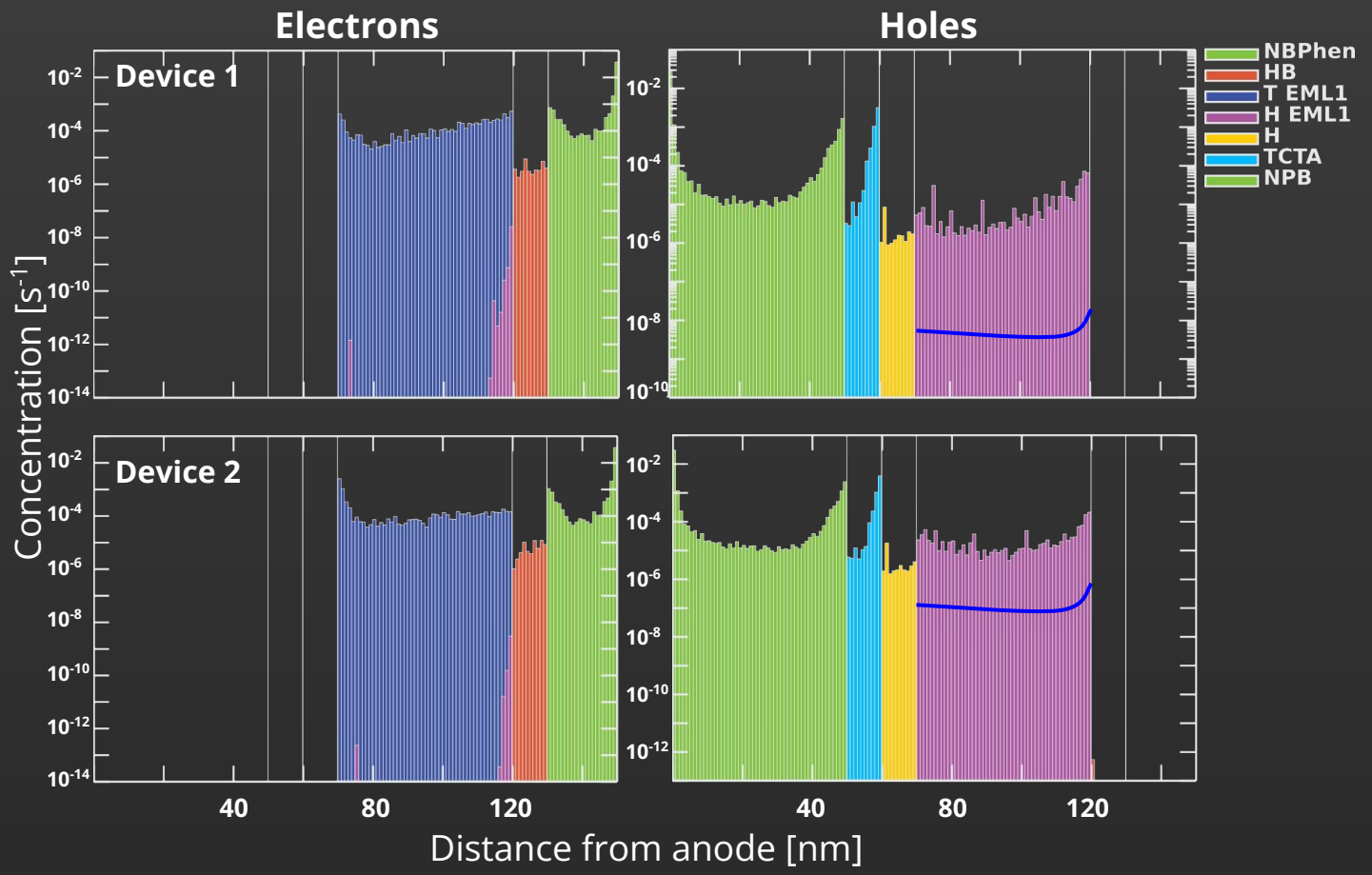
- **IP (HOMO) values**: fair agreement between predicted and experimental results
- **EA (LUMO) values**: differences between calculated and experimental results due to an inconsistent consideration of the exciton binding energy in conventional EA experiments
- **Excitonic energies**: fair agreement between predicted (2.59) and experimental (2.65) singlet energy of T molecule
- **Ordering** of the exciton energies as expected





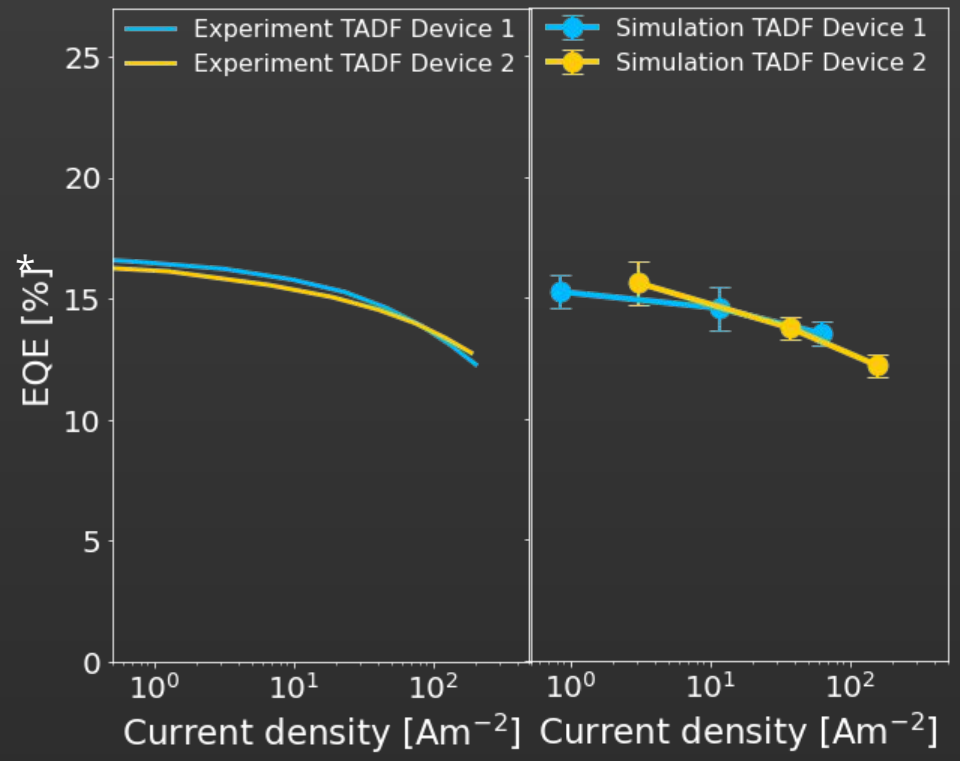
Device level predictions – TADF

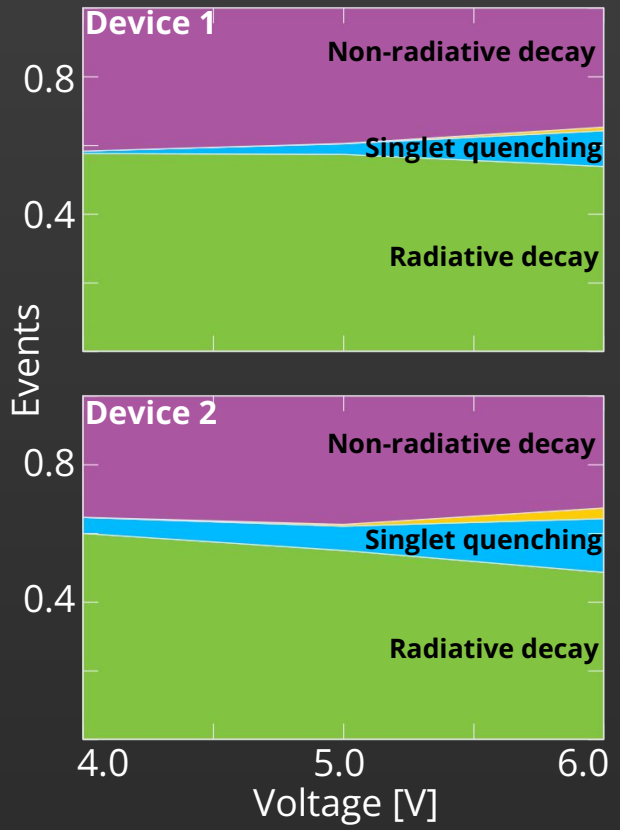




- Increasing T concentration in emission layer (EML) increases overall current density
- Fair prediction of *J*(*V*)

Device level predictions – TADF





- Excellent prediction of the EQE
- Main loss mechanisms: Non-radiative decay & singlet quenching, occurring mostly on T molecules
- Emission of the device is exclusively from T molecules

* 25 % outcoupling efficiency is assumed

HF devices

EML concentrations:

- Device 1: 0.7 mol% F, 9.3 mol% T, 90 %mol H
- Device 2: 0.7 mol% F, 20.0 mol% T, 79.3 %mol H

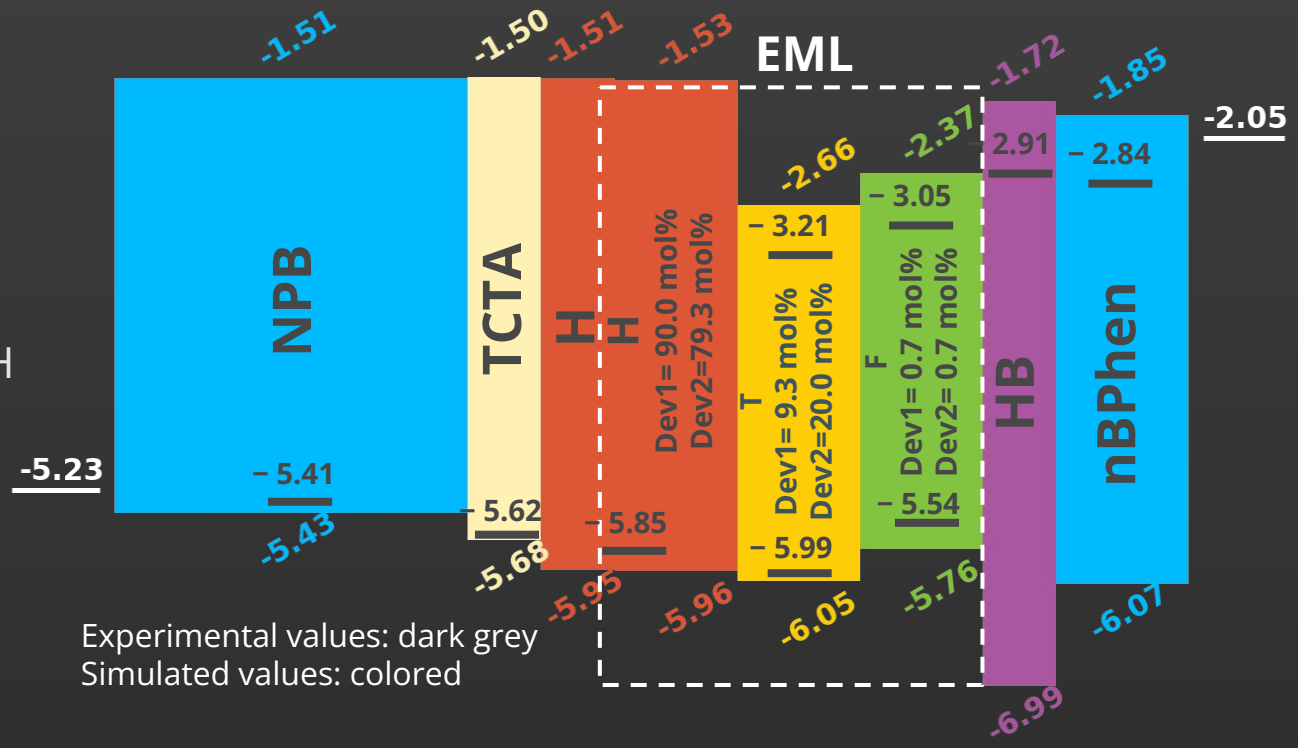
Task of the case study:

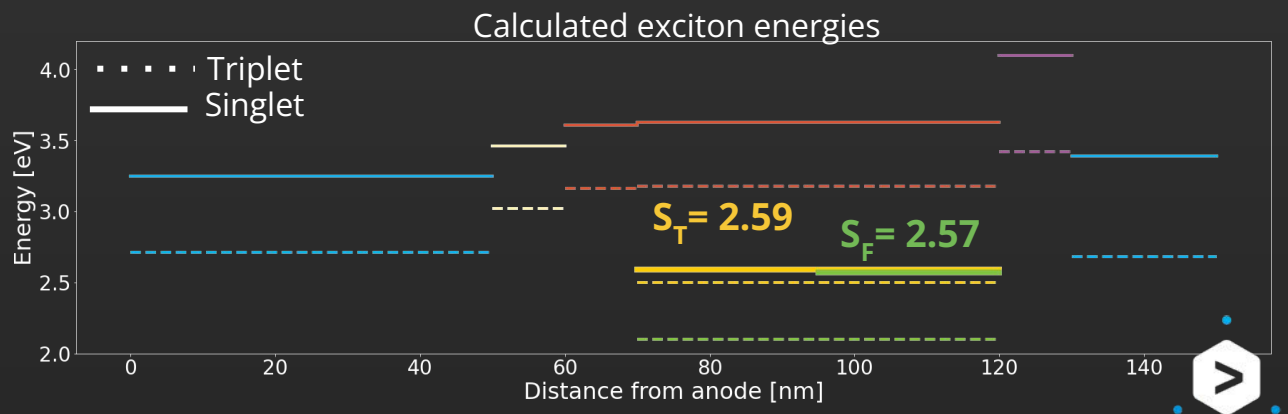
Trend analysis of *J*(*V*) and EQE of HF devices with different host-guest concentrations

Approach:

Multiscale toolchain:

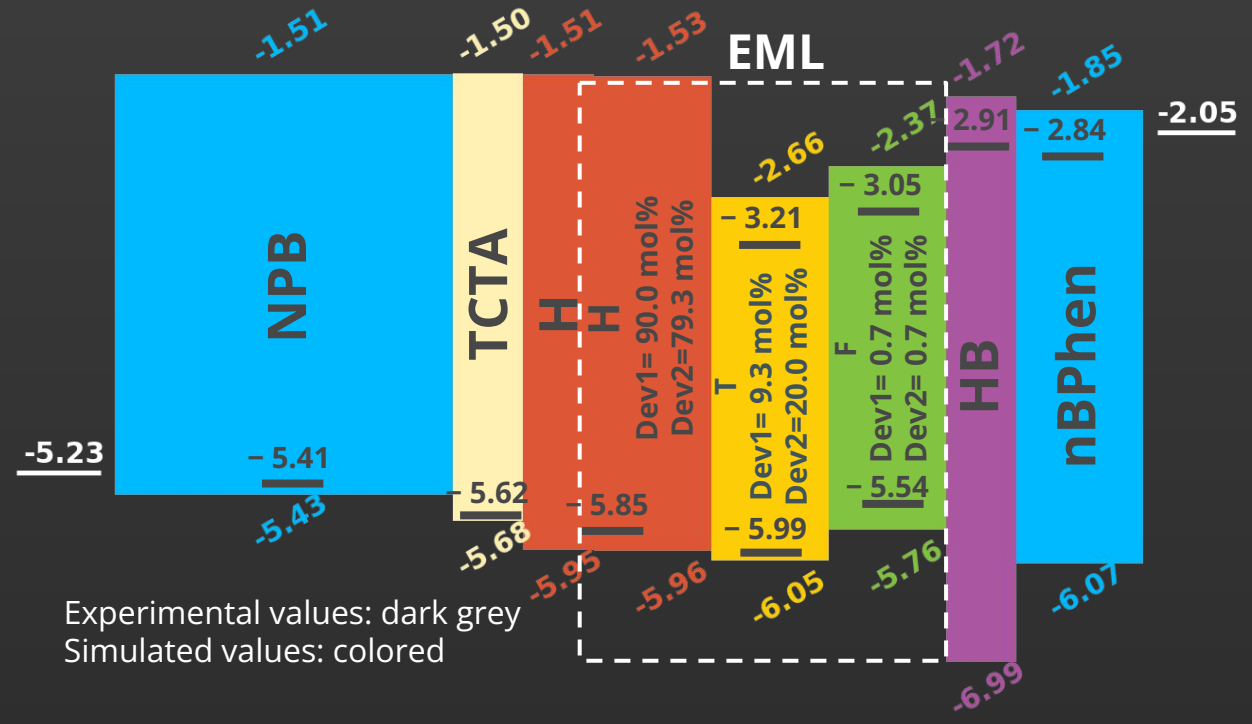
- HOMO, LUMO, and exciton energies
- Up to device performance

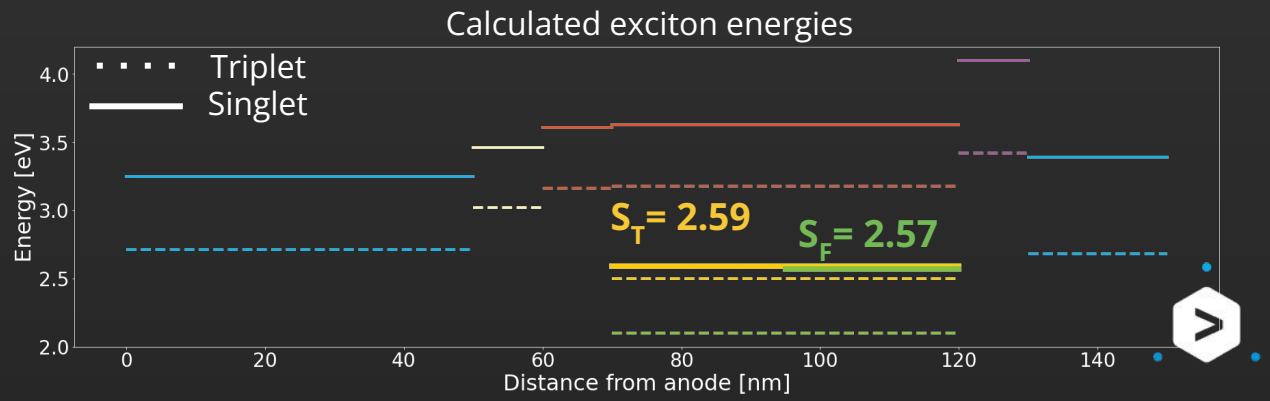




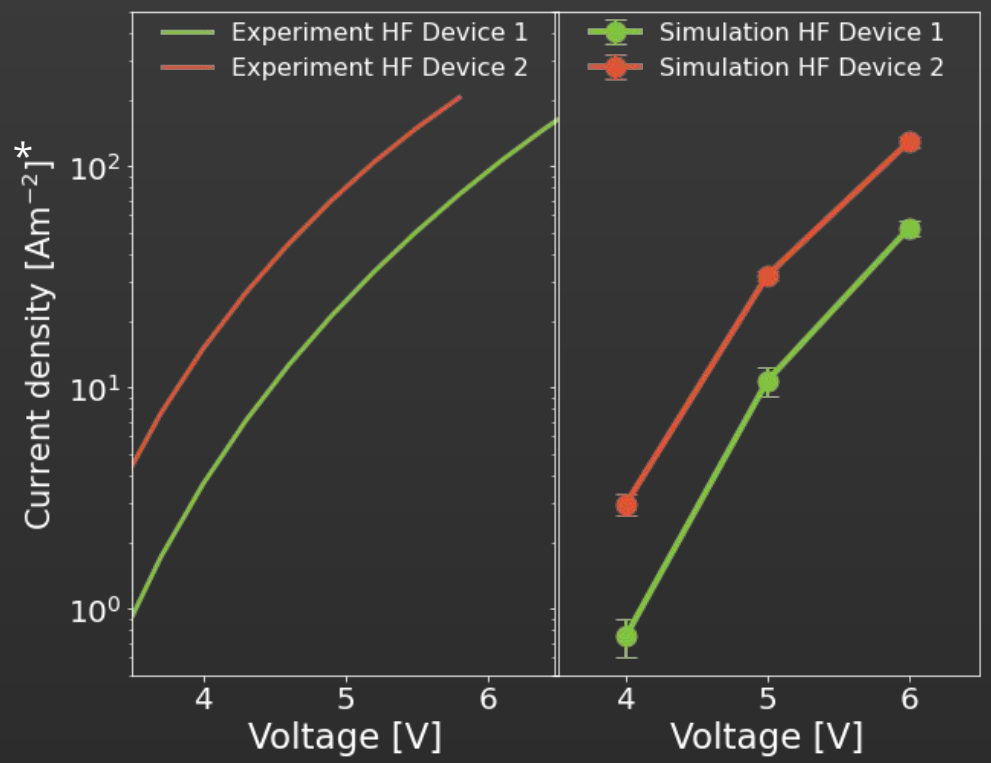
Molecular scale predictions – HF

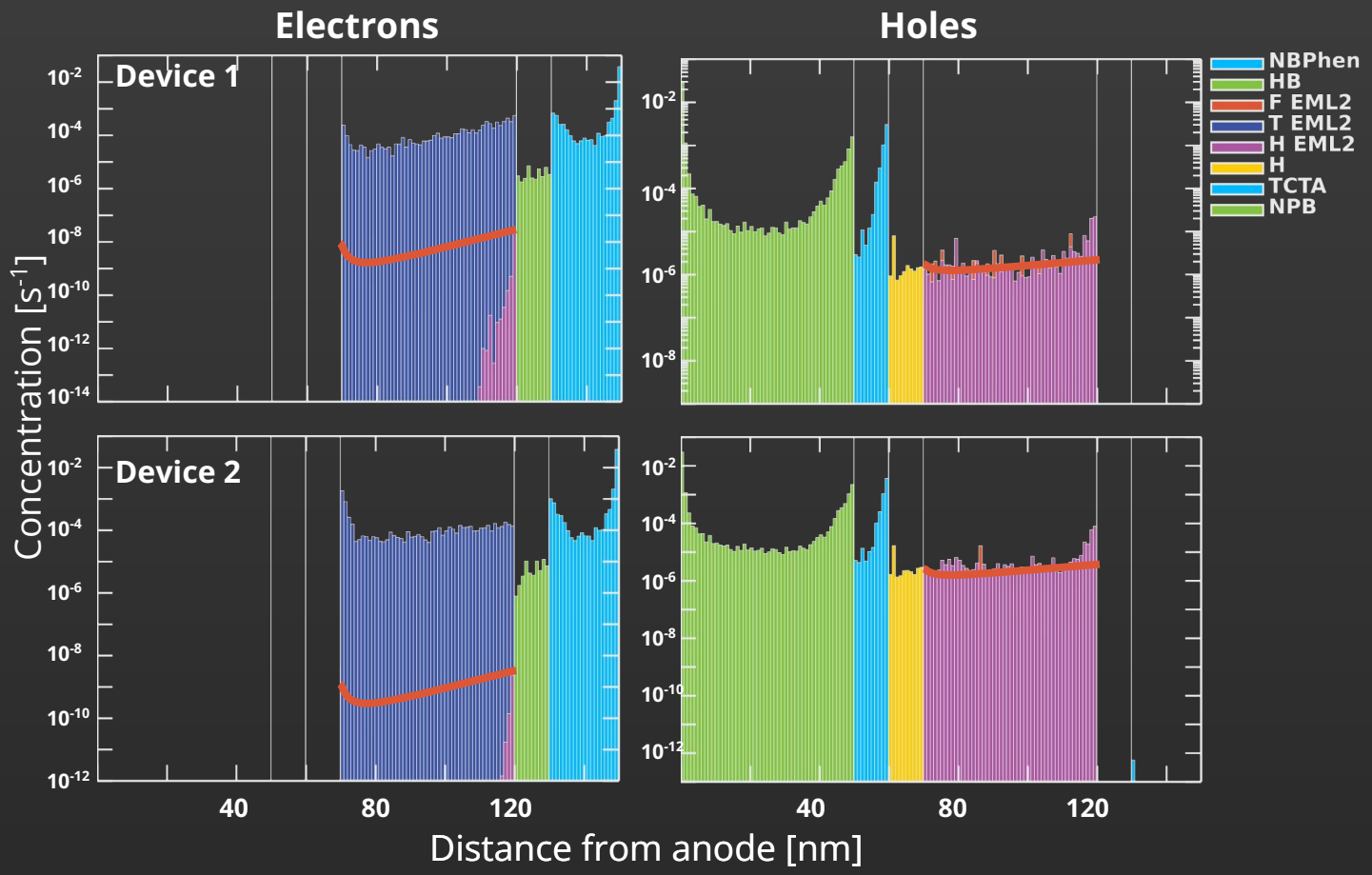
- **HOMO and LUMO values**: similar conclusions as for the TADF stack. Ordering of the energy levels is consistent.
- **Excitonic energies**: fair agreement between predicted (2.57 eV) and experimental (2.45 eV) singlet energy of F molecule.
- **Ordering** of the exciton energies as expected





Device level predictions - HF

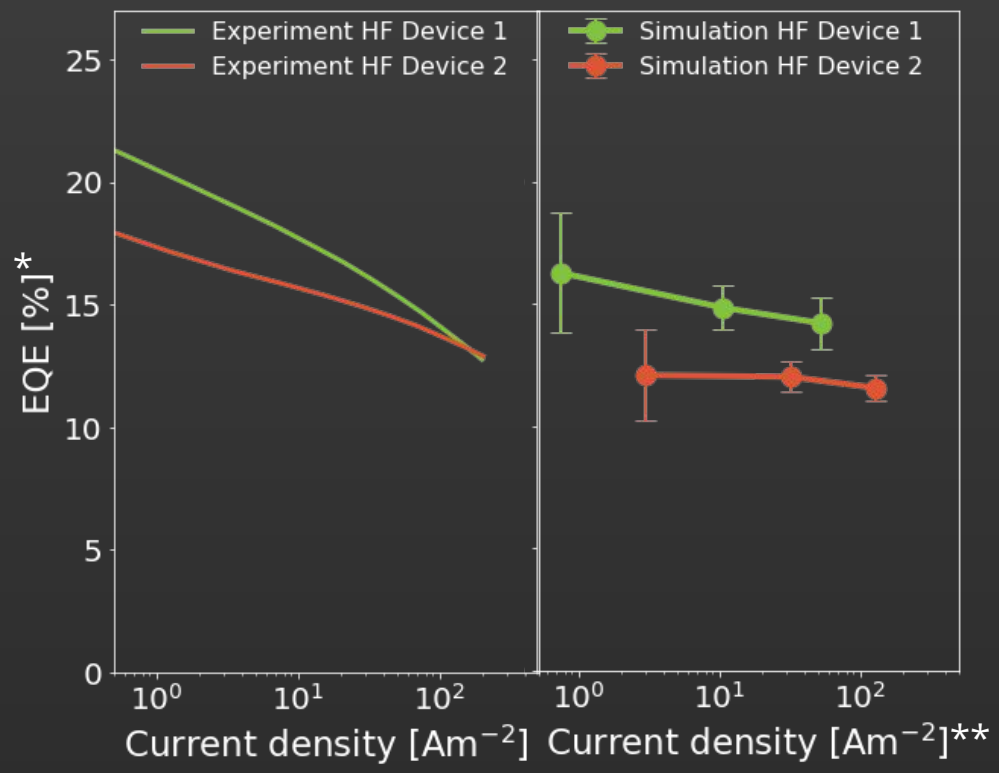


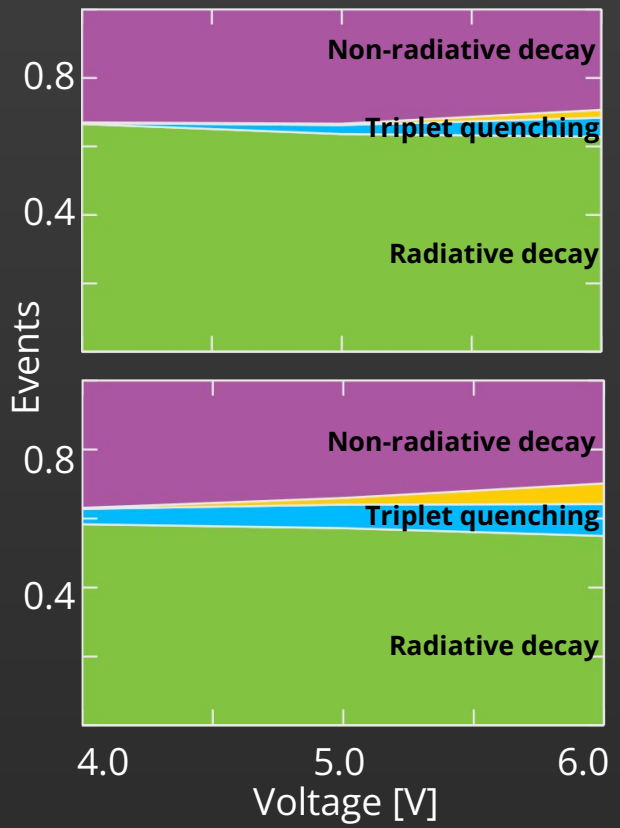


- Increasing T concentration in the emission layer (EML) increases the overall current density
- Fair prediction of the *J*(*V*)

* It is assumed that the mobility of F molecule is lower than other molecules in the device

Device level predictions - HF





- The experimental trend in the EQE is very well predicted
- Non-radiative decay and triplet quenching are the main loss mechanism that occur mostly on the F molecules
- The emission of the device is exclusively from the F molecules.

* 25 % outcoupling efficiency is assumed
** It is assumed that the mobility of F molecule is lower than other molecules in the device

Demo time (Simbeyond)

Summary and conclusions

- Our multiscale toolchain developed with SCM allows to explore the device level properties of OLEDs without the need of experimental input parameters
- Our toolchain is now operational and validated for electronic and excitonic trend predictions
- It is also possible to extend our toolchain with the other features of Bumblebee such as device degradation scenarios and lifetime prediction of the OLEDs

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Backup slides

Overview of simulation methods

	1D Drift Diffusion	3D Master Equations	3D Kinetic Monte Carlo
Overall Accuracy	−	+	++
Simulation speed	++	+	~
Charge transport	~	+	++
Excitonic processes	~	+	++
Complex device structures	−−	+	++
Input parameters/ Simulation workflow	~	++	++
Predictiveness	~	+	++

Overview of collaboration possibilities

Simbeyond's product and service portfolio

Software & support

Bumblebee Licenses & Services (1+ months)

- Bumblebee License Units
- Additional modules
- Technical support
- Local support

Knowledge & Training

Masterclass
Interactive workshop
Training program

- Bumblebee training & results
- Direct hands-on support
- Lectures and interactive Q&A
- Bumblebee License Units
- Additional modules

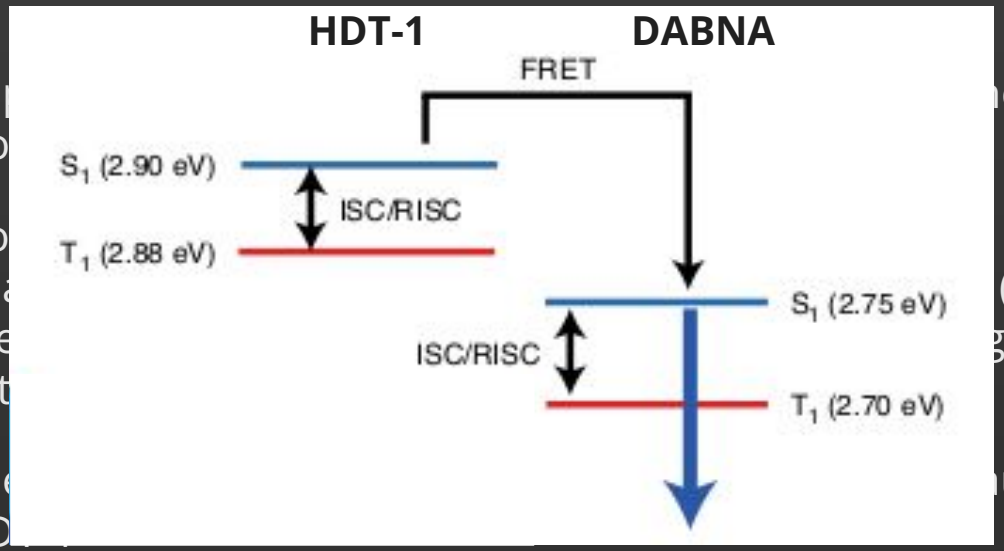
Consultancy & Projects

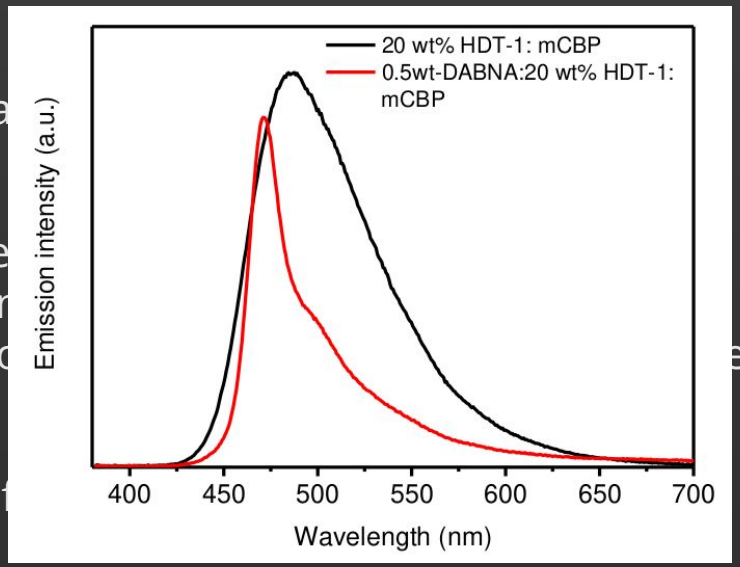
On-demand expertise
Project in cooperative mode
Project outsourced to Simbeyond

- OLED material and device experts
- Direct hands-on support
- Local support & consultancy
- Bumblebee License Units
- Additional modules

Molecular scale predictions

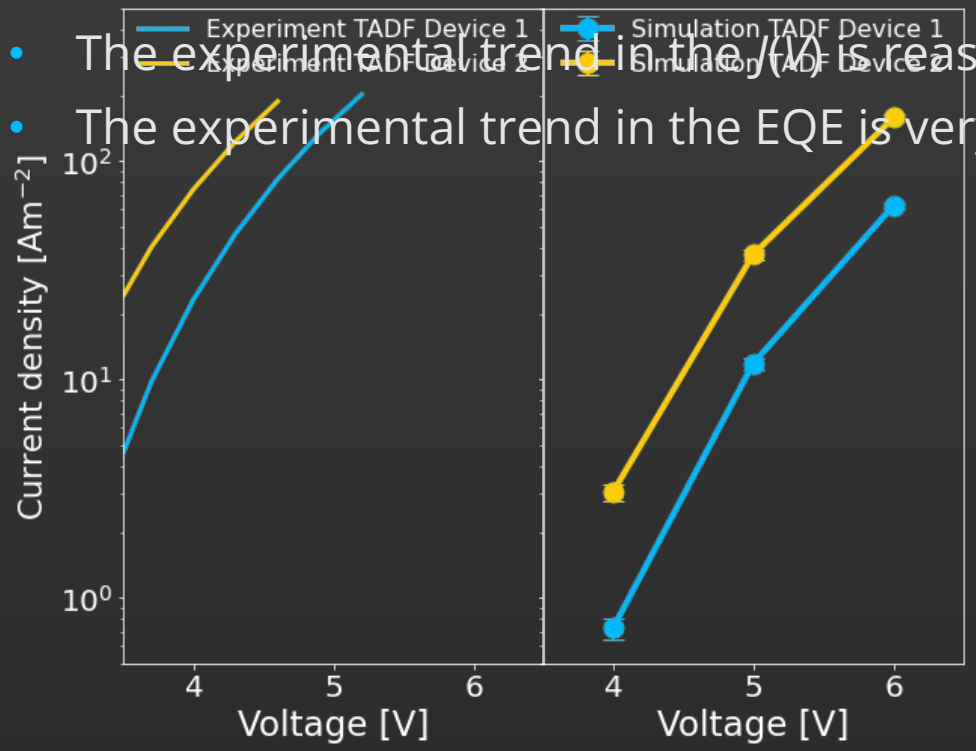
- Pa… …er tha… …fro…
- Ho… …in the… …(bl… …(red i… …the… …gths (lo… …e …wit…
- The… …use of… …HD…

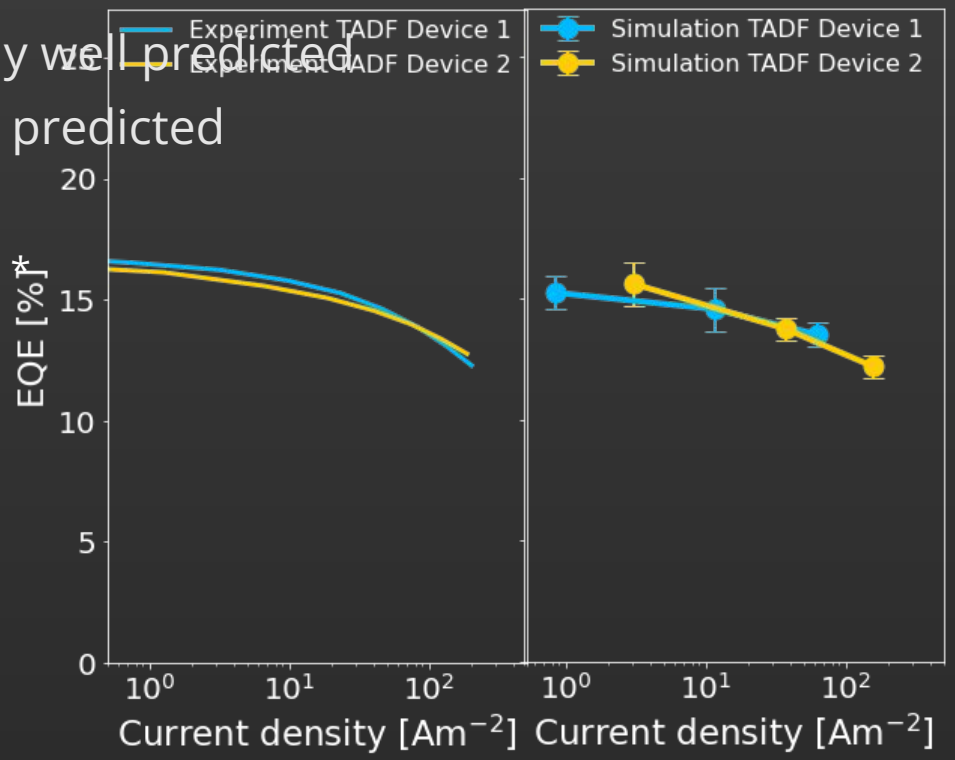




Device level predictions – TADF

- The experimental trend in the *JV* is reasonably well predicted
- The experimental trend in the EQE is very well predicted

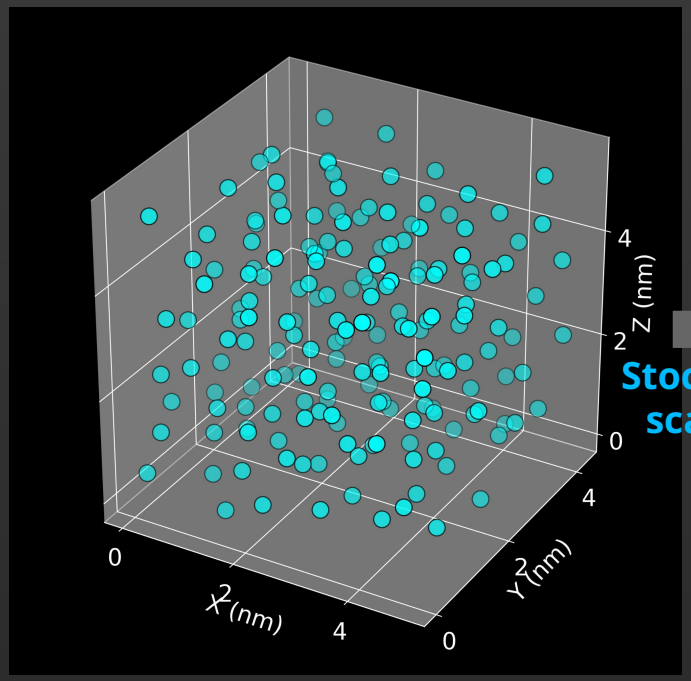




* 25 % outcoupling efficiency is assumed

Morphology scaling

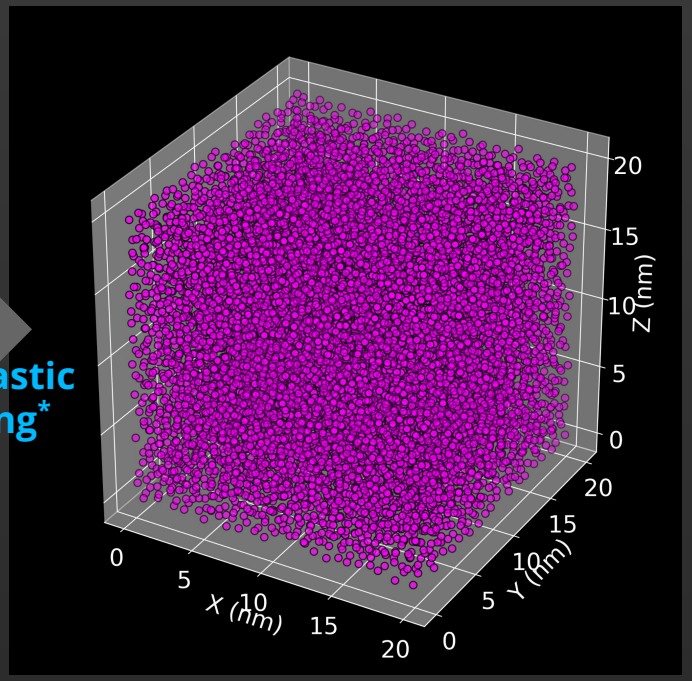
Deposition box



4.95 × 4.29 × 5.37 nm³
184 molecules,
n = 1.61 molecule/nm³
min. NN dist = 0.59 nm

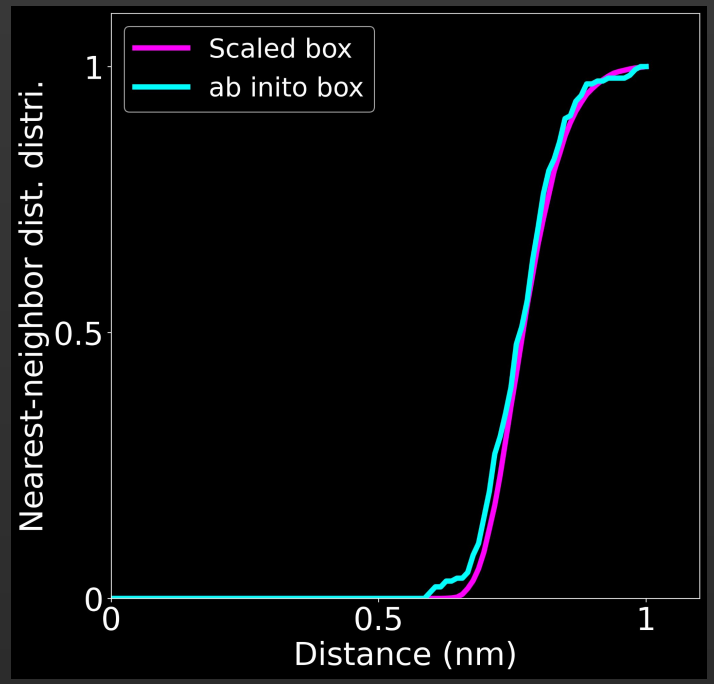
Stochastic scaling*

Scaled box



20 × 20 × 20 nm³
12841 molecules,
n = 1.60 molecule/nm³
min. NN dist = 0.62 nm

Nearest-neighbor (NN) distance distribution comparison



Good agreement in NN distance distribution

* Baumeier et al. PRB **86**, 184202 2012)

Opportunity: simulation-assisted approach

Our 3D Kinetic Monte Carlo approach enables to go beyond the conventional trial-and error approach: