

OLED Device Simulation with Quantum Chemistry and Kinetic Monte Carlo Simulations

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Why?

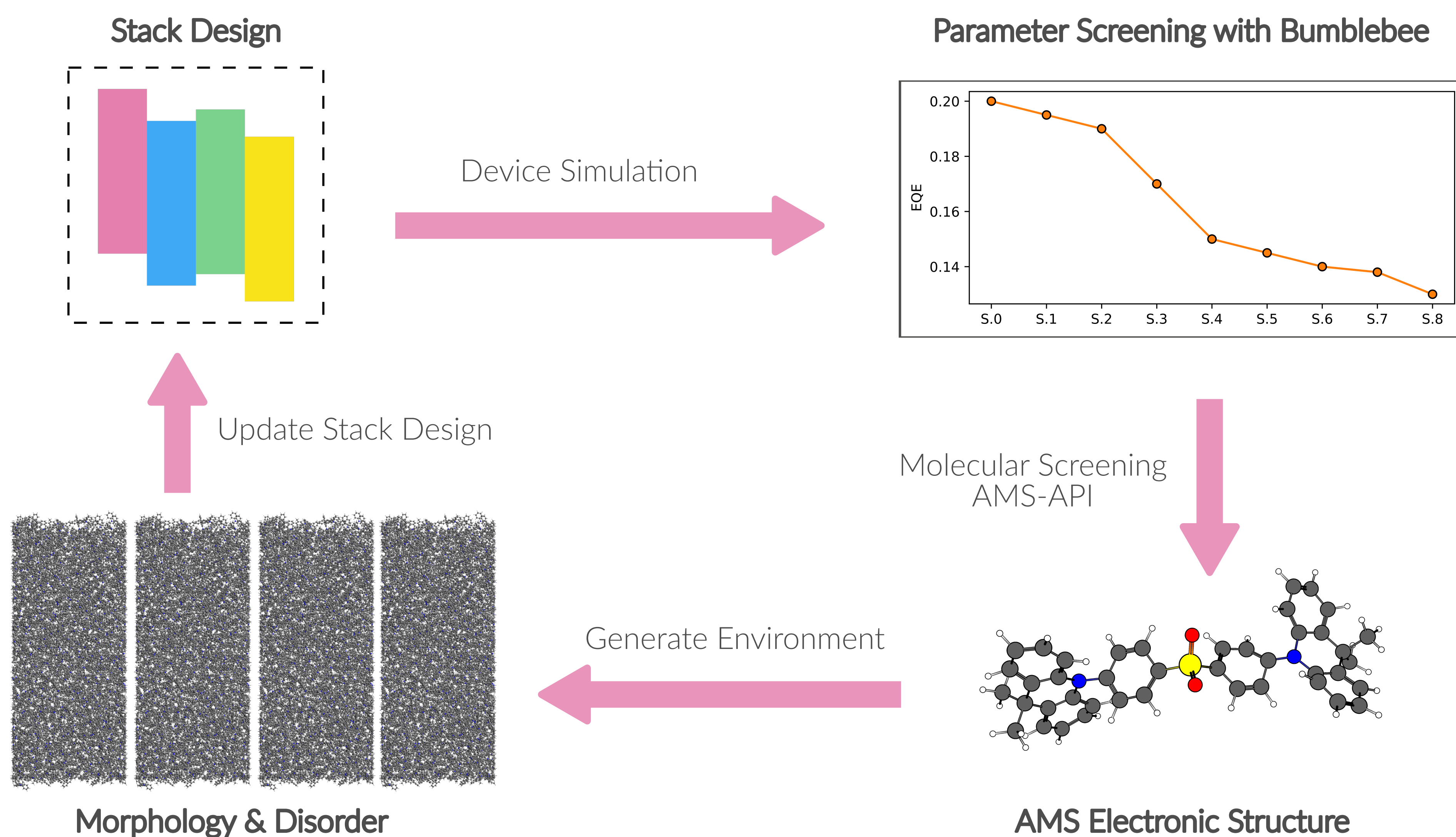
Complex processes and degradation mechanisms limit OLED efficiency and lifetime.

Simulation links material properties to device performance for faster, cost-effective OLED optimization.



bumblebee
OLED device simulations reimagined

Multiscale Simulation for OLED Design

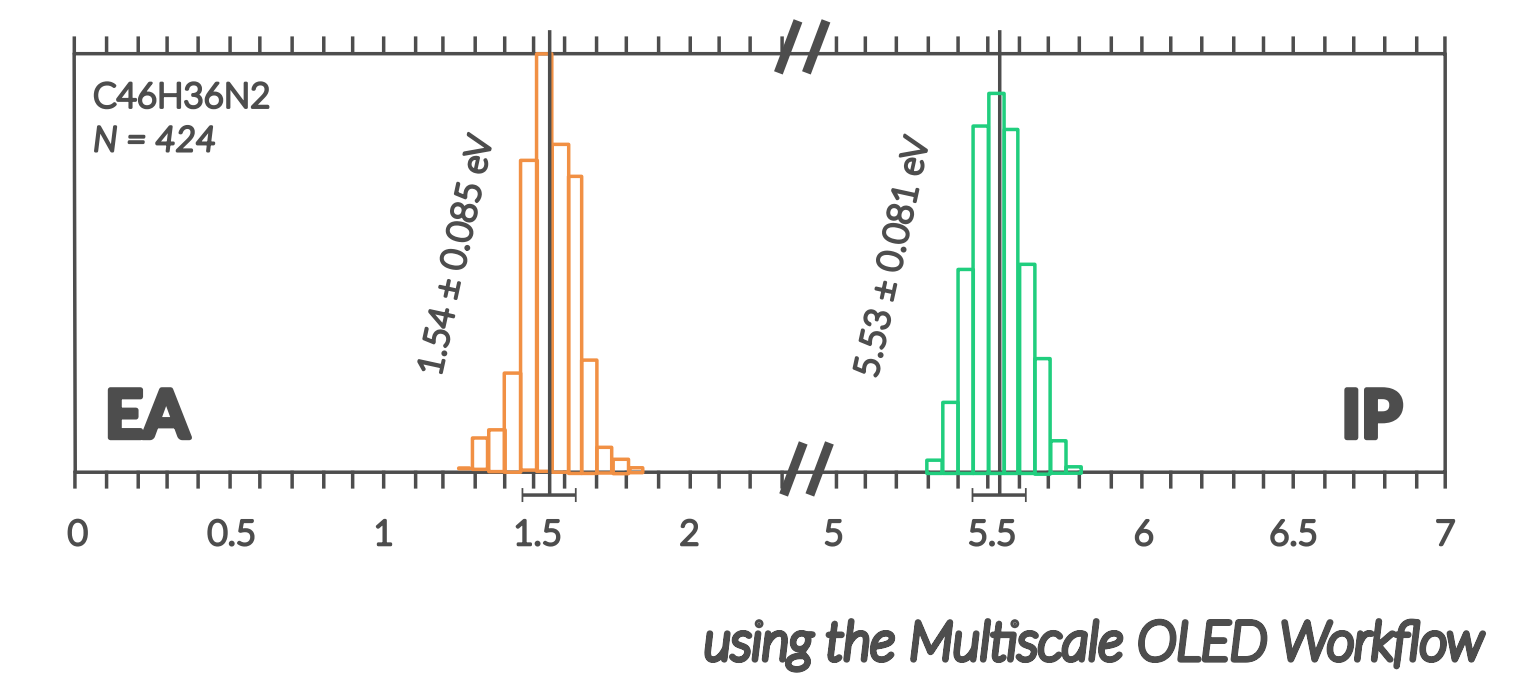


- Combines quantum mechanical calculations (AMS) with 3D kinetic Monte Carlo simulations (Bumblebee)
- Enables modeling of charge transport, exciton dynamics, degradation, and optical outcoupling
- Supports optimization of OLED efficiency, lifetime, and performance
- Quantify the effect of trap states, SOP, TTA and TPQ

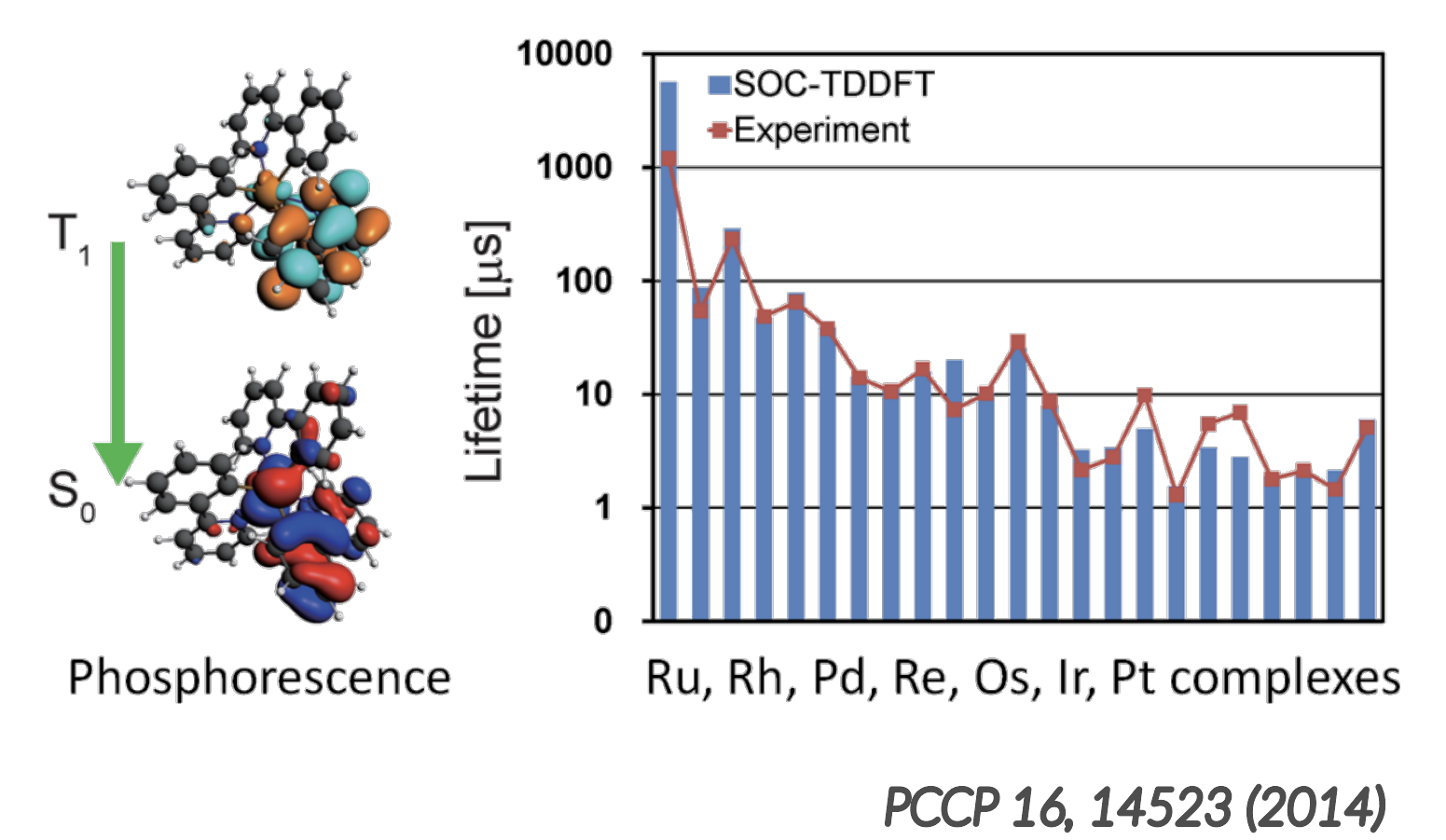
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AMS Electronic Structure

Electron Affinities and Ionization Potentials

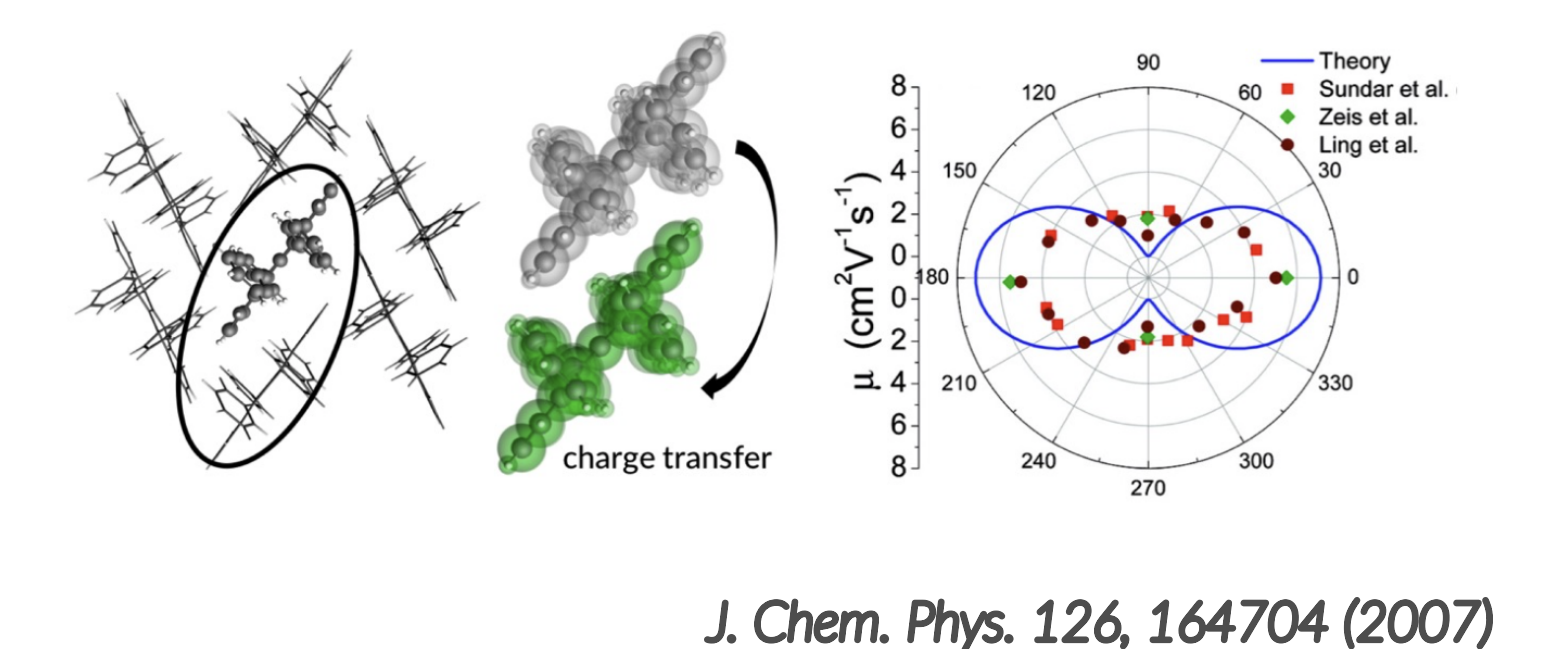


Optimize OLED Emitter Lifetimes



PCCP 16, 14523 (2014)

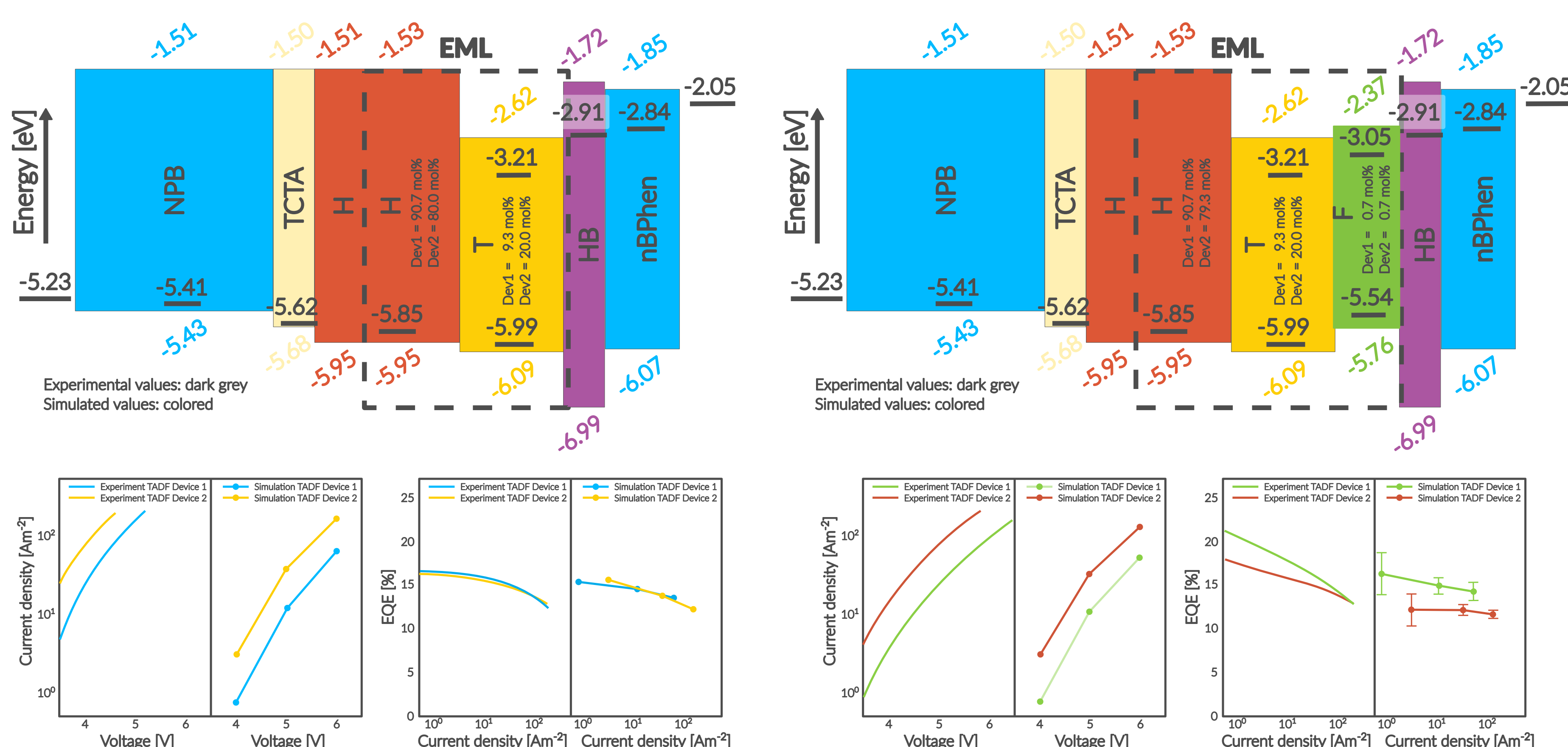
Optimize Charge Mobility



J. Chem. Phys. 126, 164704 (2007)

Pilot Study with Cynora

Simulated impact of host-guest doping on J(V) and EQE in TADF and HF devices.

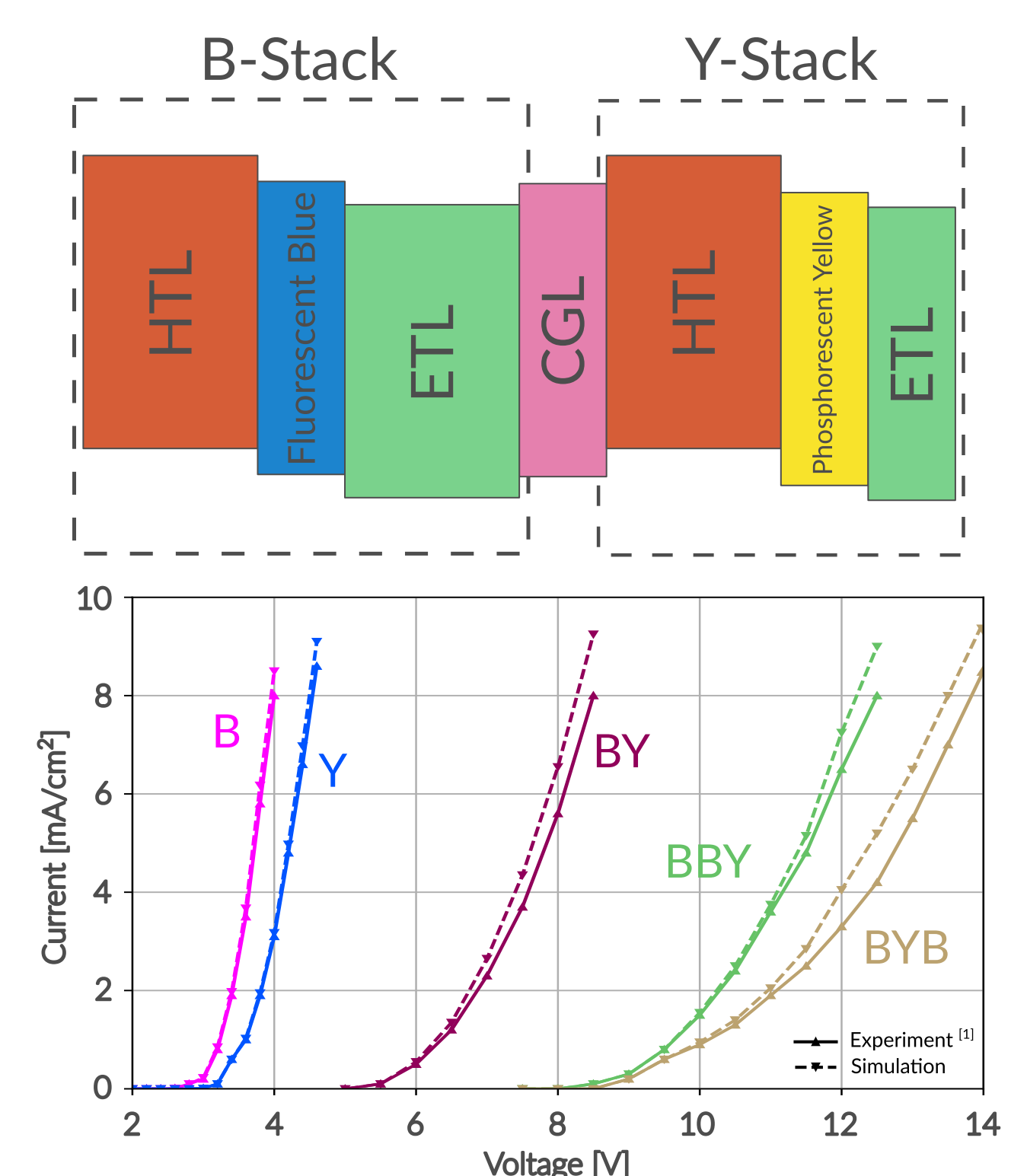


Results

- Excellent qualitative and good quantitative agreement with experiment
- 3D KMC results provide insight into the percolative transport of electrons and holes, selective emission processes, and the main degradation pathways and loss mechanisms
- Improve performance through rational design at the material and stack levels
- Test virtually to save precious lab resources

Tandem Stacks

Design tandem and multi-stack devices



- Optimize interfaces
- Position-resolved angular emission spectra

[1] Optics Express 24, 28131 (2016)

Scan to Watch: 20 minute introduction

