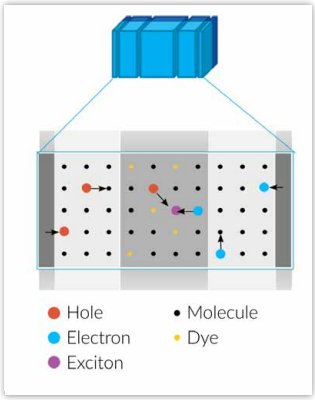
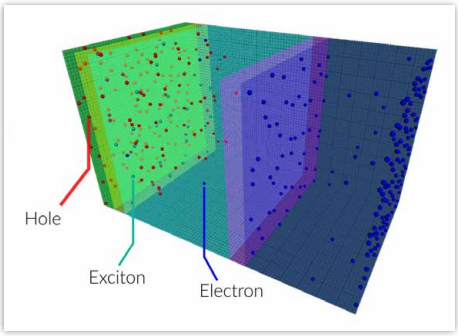
OLED device modeling - Bumblebee

3D-kMC simulation tool for OLED stacks

Bumblebee is a simulation tool used to model the long-term behavior of OLED materials by tracking the diffusion of carriers, molecular emissions and device degradation over time. It helps researchers understand how defects form, how materials age, and how charge carriers move within OLED layers, crucial for improving device efficiency and lifespan.



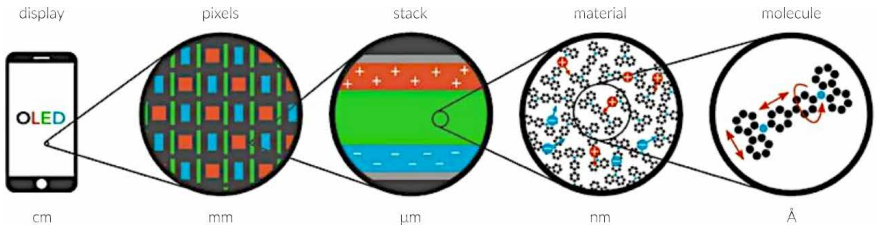


Use Bumblebee to

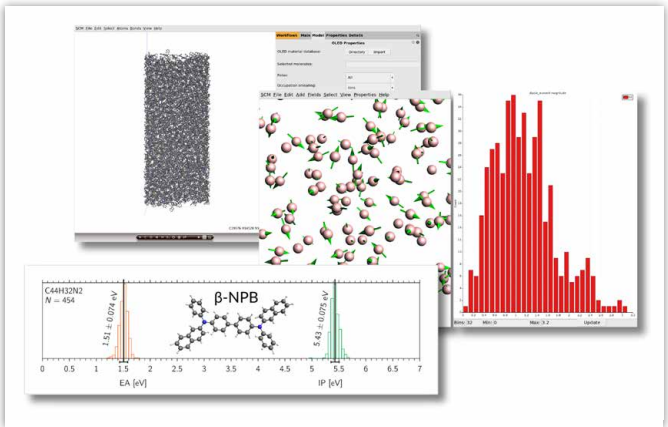
- Model state-of-the-art OLED materials including TADF emitters and hyperfluorescence
- Locate processes in your stack thanks to explicit morphologies and time-evolution
- Model host-guest distributions, layer interfaces, dopant gradients, polymer networks and other complex structures
- Include complex opto-electronic processes: exciton annihilation, polaron quenching, triplet harvesting, exciplexes, vibronic coupling, and more
- Include molecular disorder and long-range electrostatic interactions
- Optical outcoupling for light management
- New algorithms reduce computational cost by a factor 10-50 compared to standard kinetic Monte Carlo implementations
- Optimise your model with built-in parameter screening and optimisation tools

Multiscale modeling of OLED devices

First-principles OLED device simulations in combination with AMS



- Generate a realistic thin film structure via simulated physical vapor deposition
- Calculate the distribution of properties such as ionization potential, electron affinity and dipole moments for all molecules in the film
- Load properties into Bumblebee for OLED device simulations



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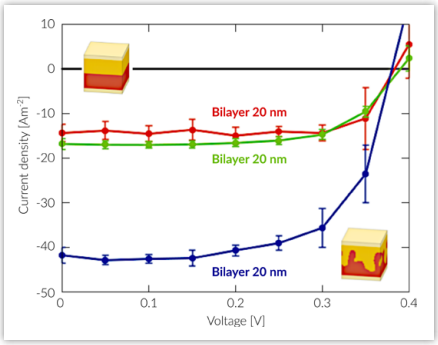
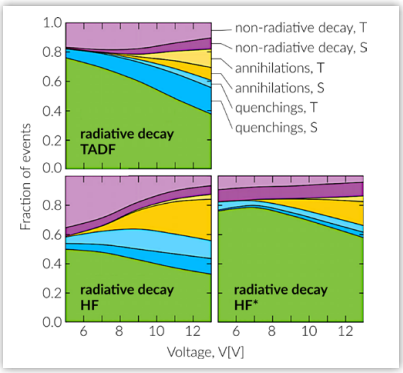
Example applications

Effect of morphology on J-V curves



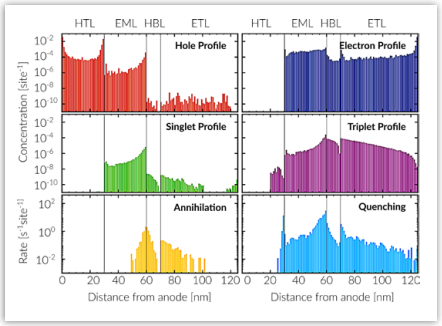
Screening of emitters and loss processes



Carrier concentrations and excitonic events per material

Inspection of the profiles:

- Charge imbalance
- Charge trapping
- Injection barriers
- Location of losses
- Exciton deconfinement
- Profiles on each material

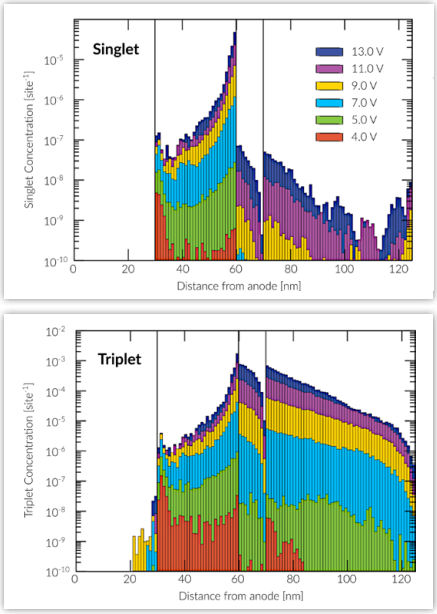


Explore Bumblebee with AMS

Excitonic profiles at different voltages

- Observe shifts in exciton localisation as charge densities change
- Identify interlayer transport limitations and blocking efficiency

mCBP/4CzIPN host-guest system (5% dye)



"What I really like about the Amsterdam Modeling Suite is that the programs were clearly written by chemists for dealing with real chemical problems. A great suite of programs!"

– Roald Hoffmann, Nobel Laureate

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