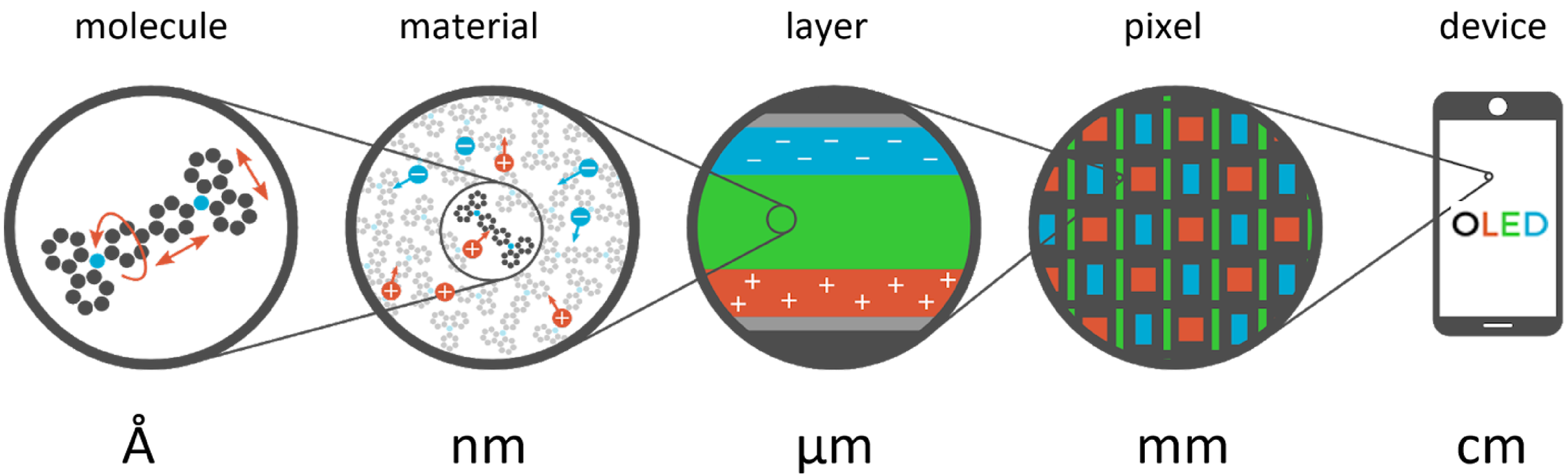
SCM
Software for Chemistry & Materials

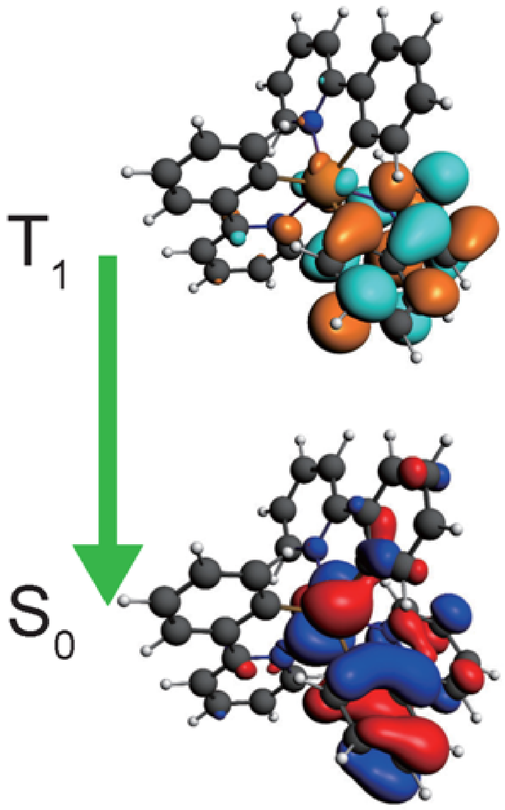
Modelling OLED: From Molecule to Device in Data-driven R&D Acceleration

Bart Klumpers, klumpers@scm.com

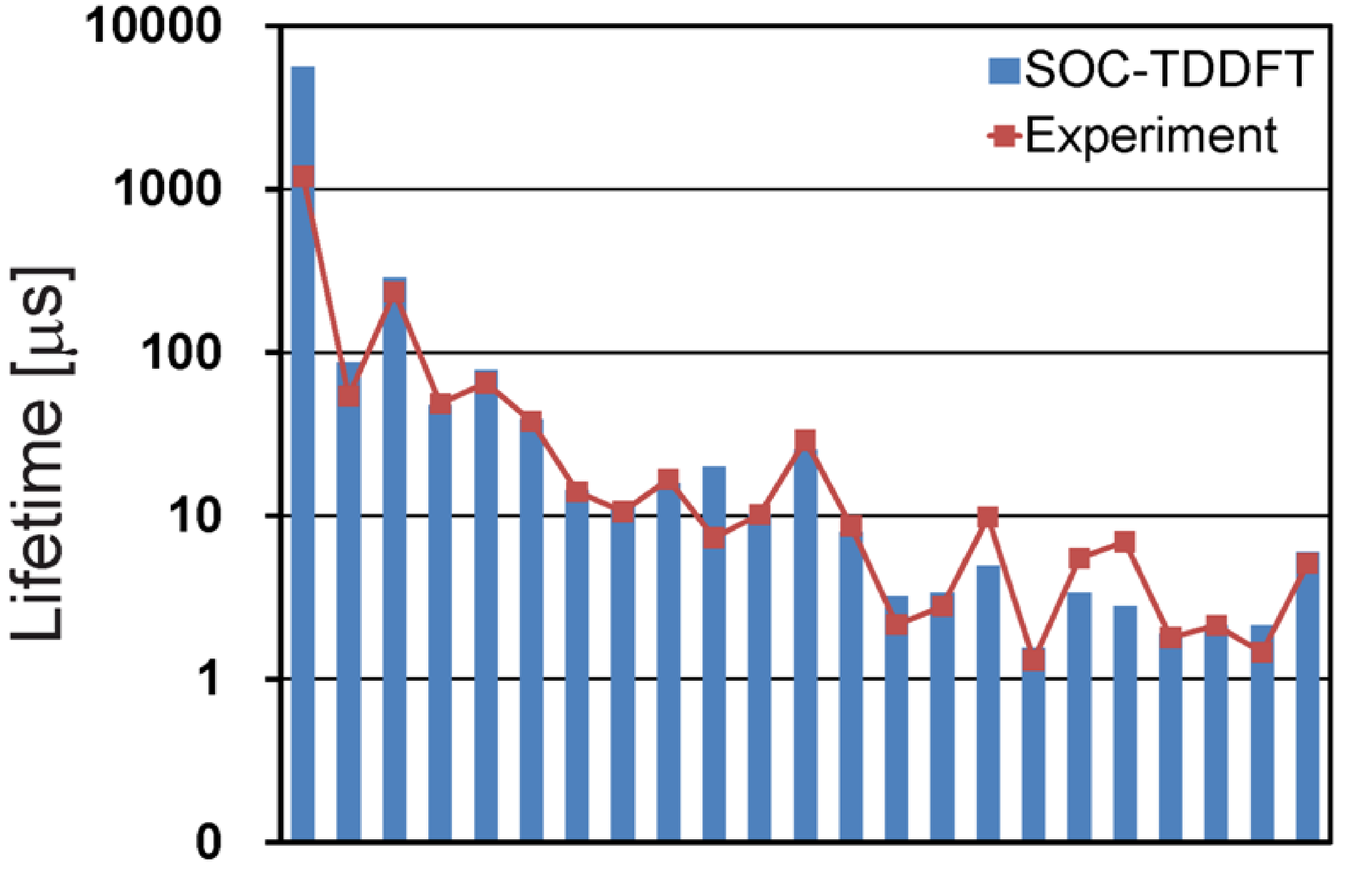
From Molecule to Device



Screening Emitter Lifetimes



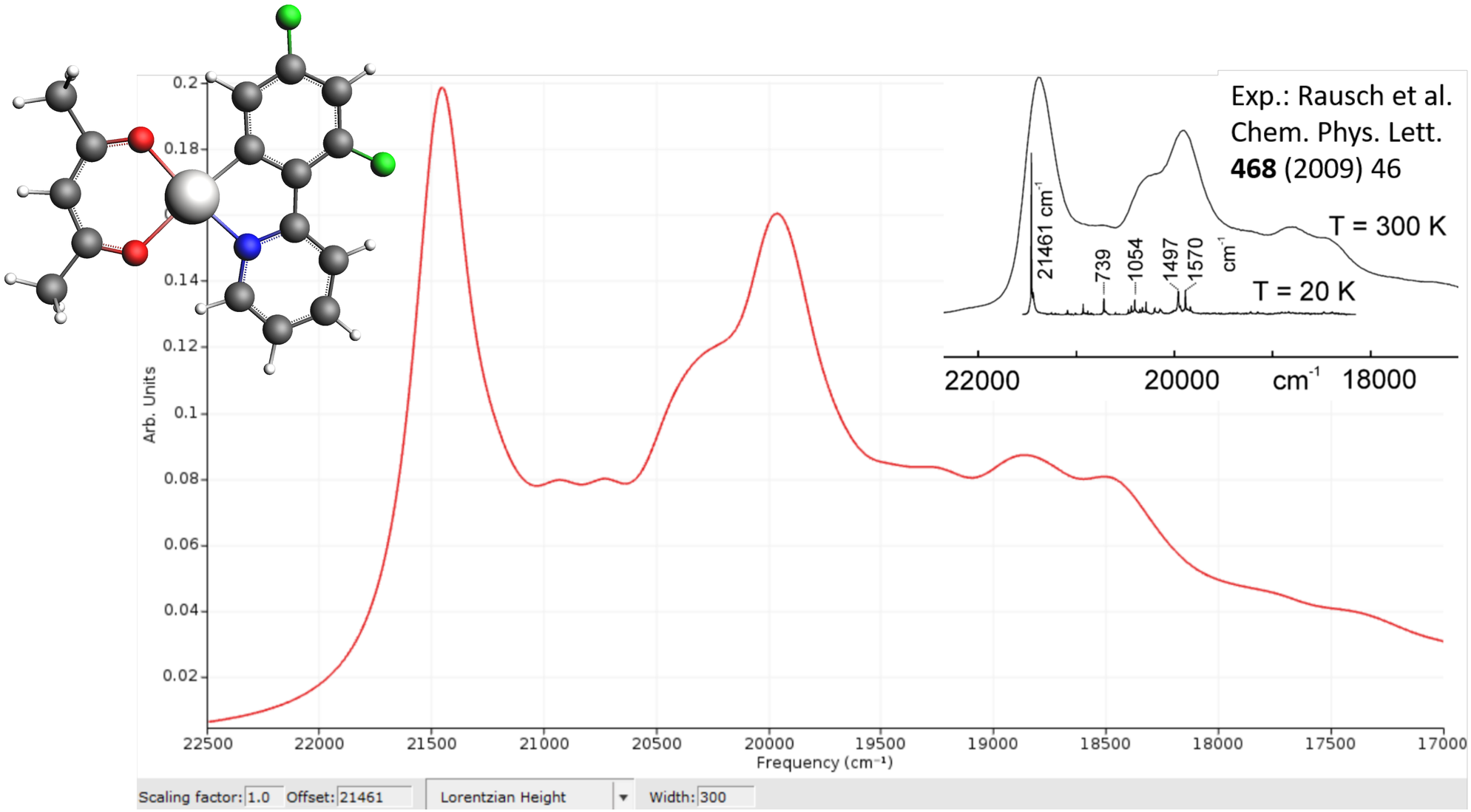
Phosphorescence



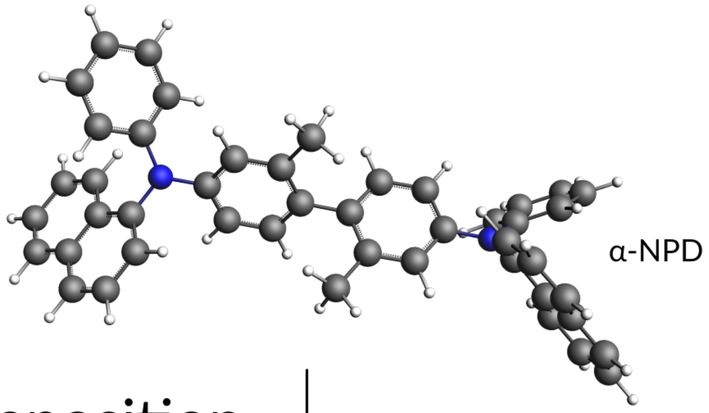
Ru, Rh, Pd, Re, Os, Ir, Pt complexes

US Patent: 20180182980

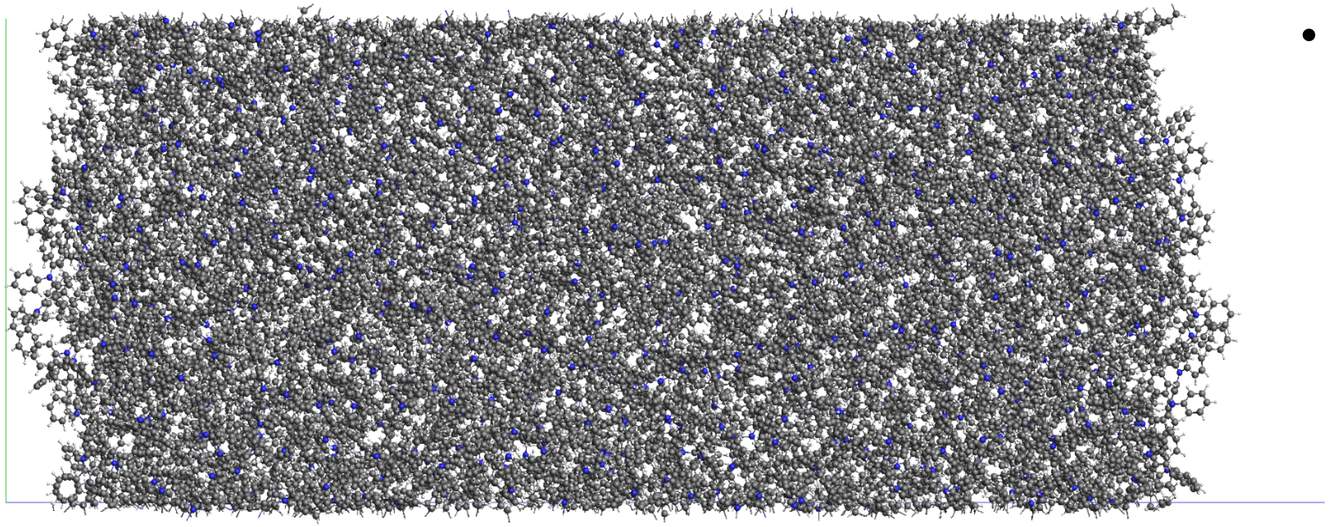
Predicting Colour Spectra



From Molecule to Layer

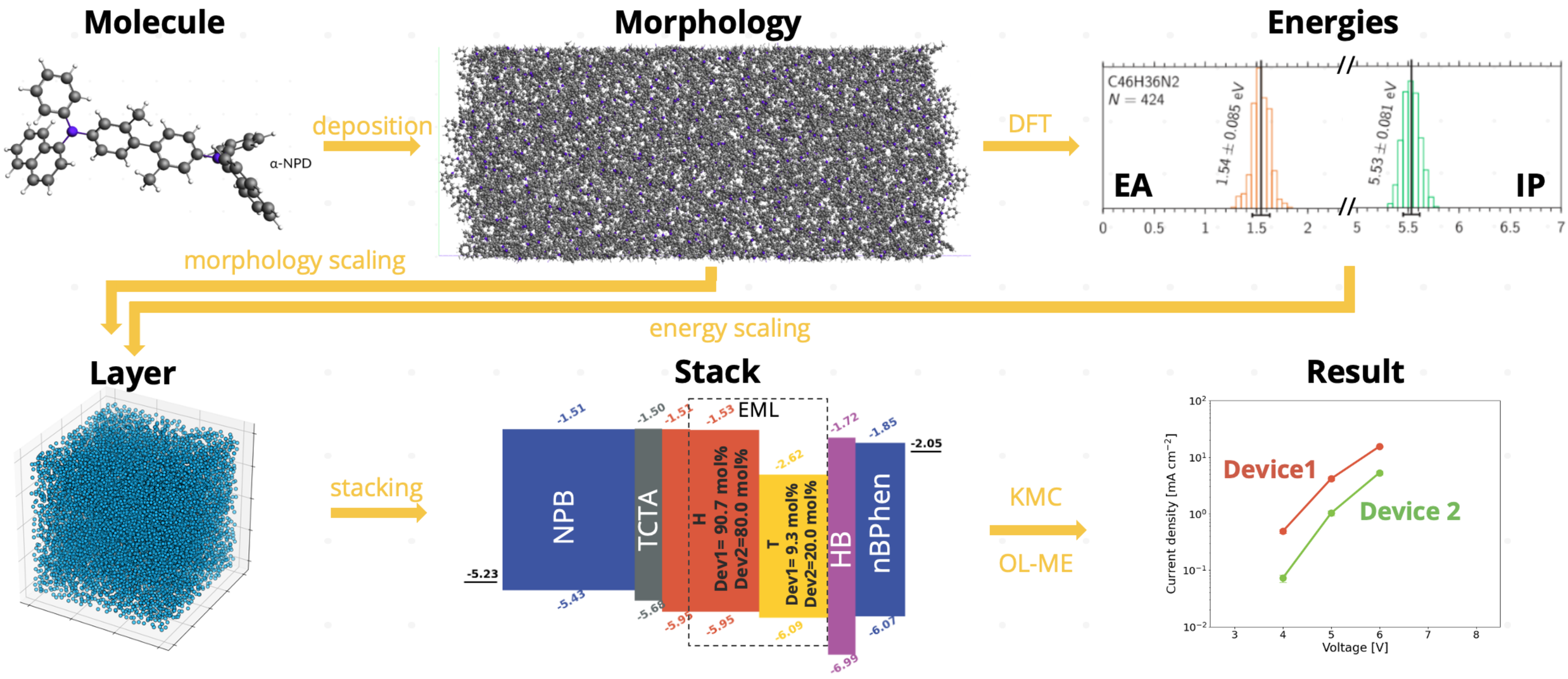


Deposition

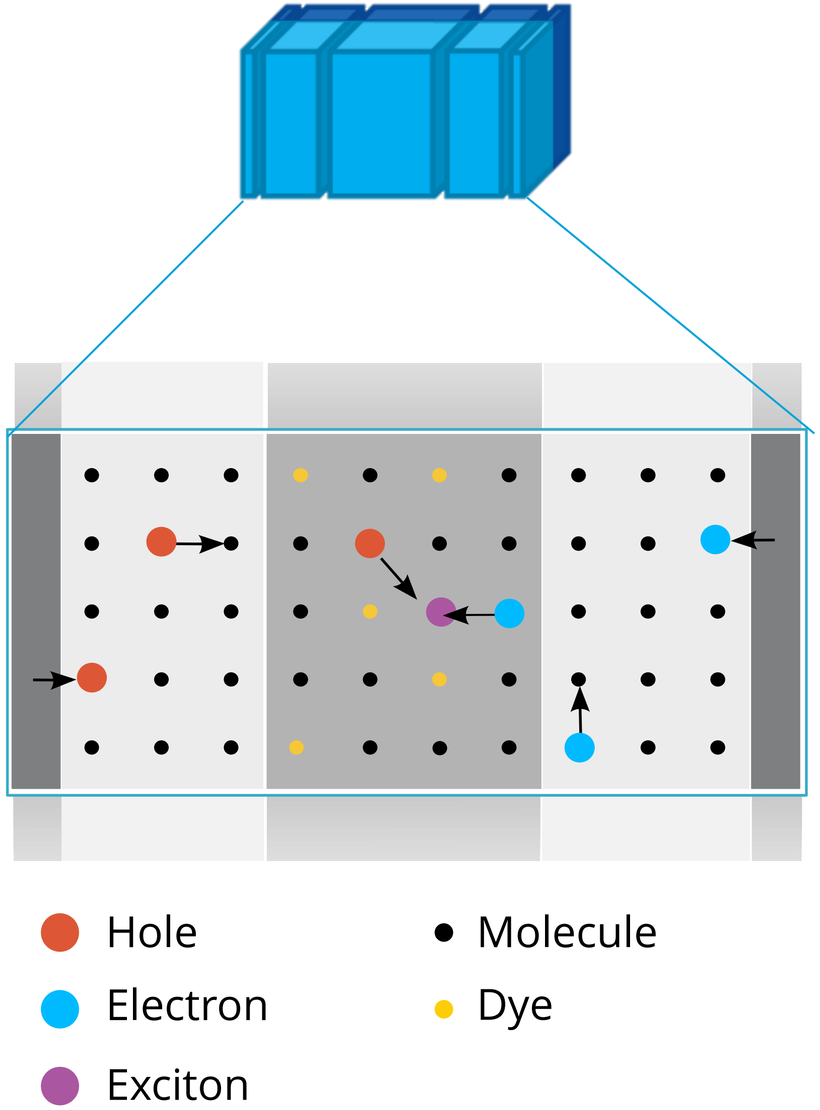


- MD Deposition
  - Explicit Morphological Disorder
  - Amorphous Environments
  - Hybrid DFT/FF
- DFT-COSMO
  - Rapid Materials Screening
  - Iterative Feed-through to the Macroscale

Multiscale Workflow

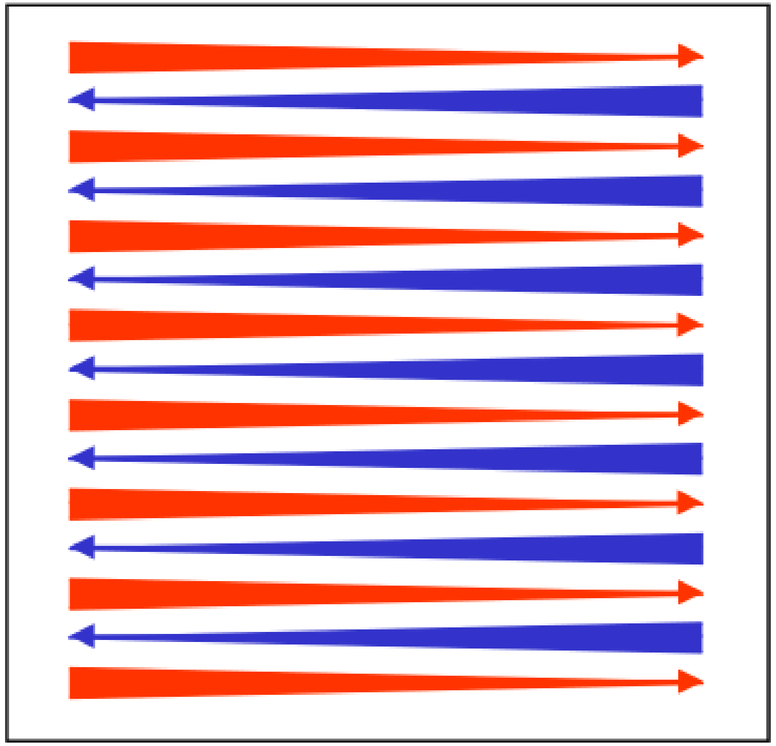


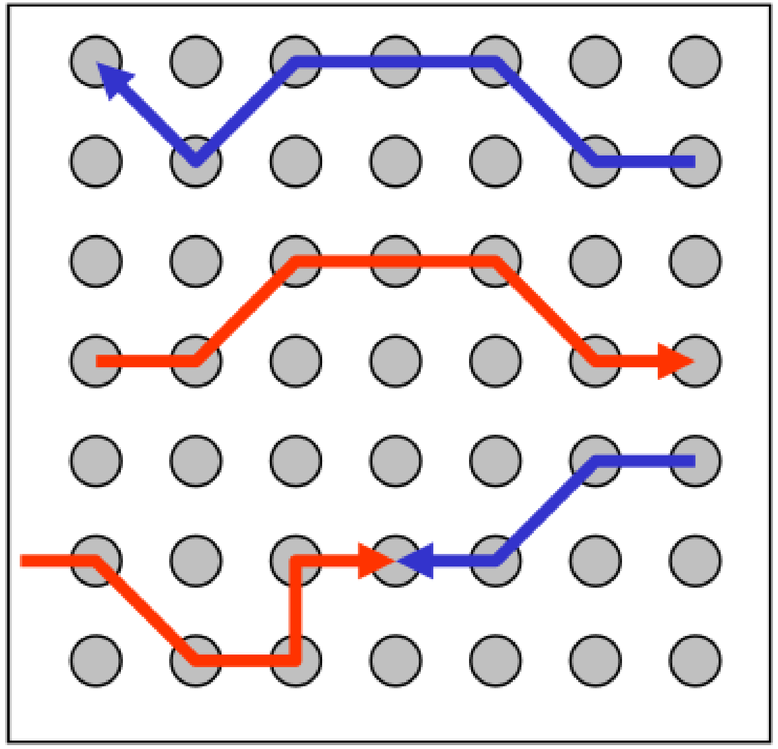
3D-kMC for OLED Stacks



- Stochastic Sampling of Electron Transport
  - Spatially Resolved
  - Diverse Exciton Interactions
  - Complex Morphologies
- Lifetime Analysis
- Small Signal Analysis
- Optical Outcoupling

Optical v. Electronic

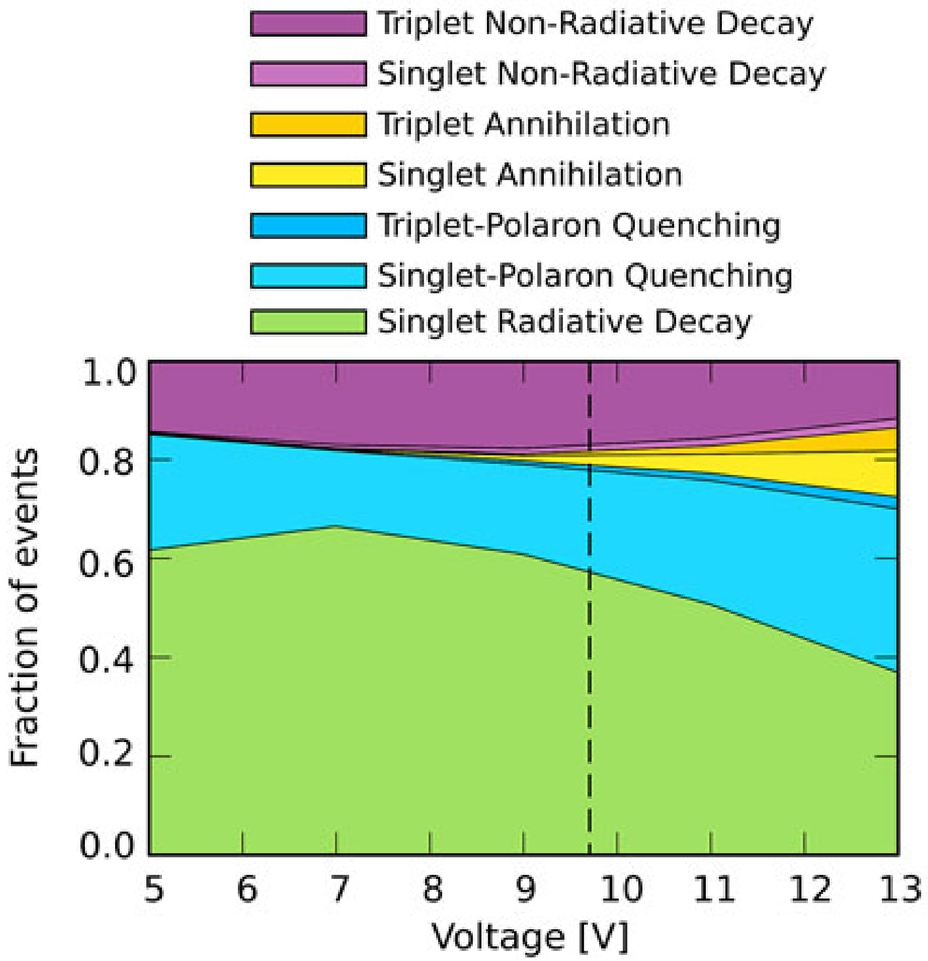


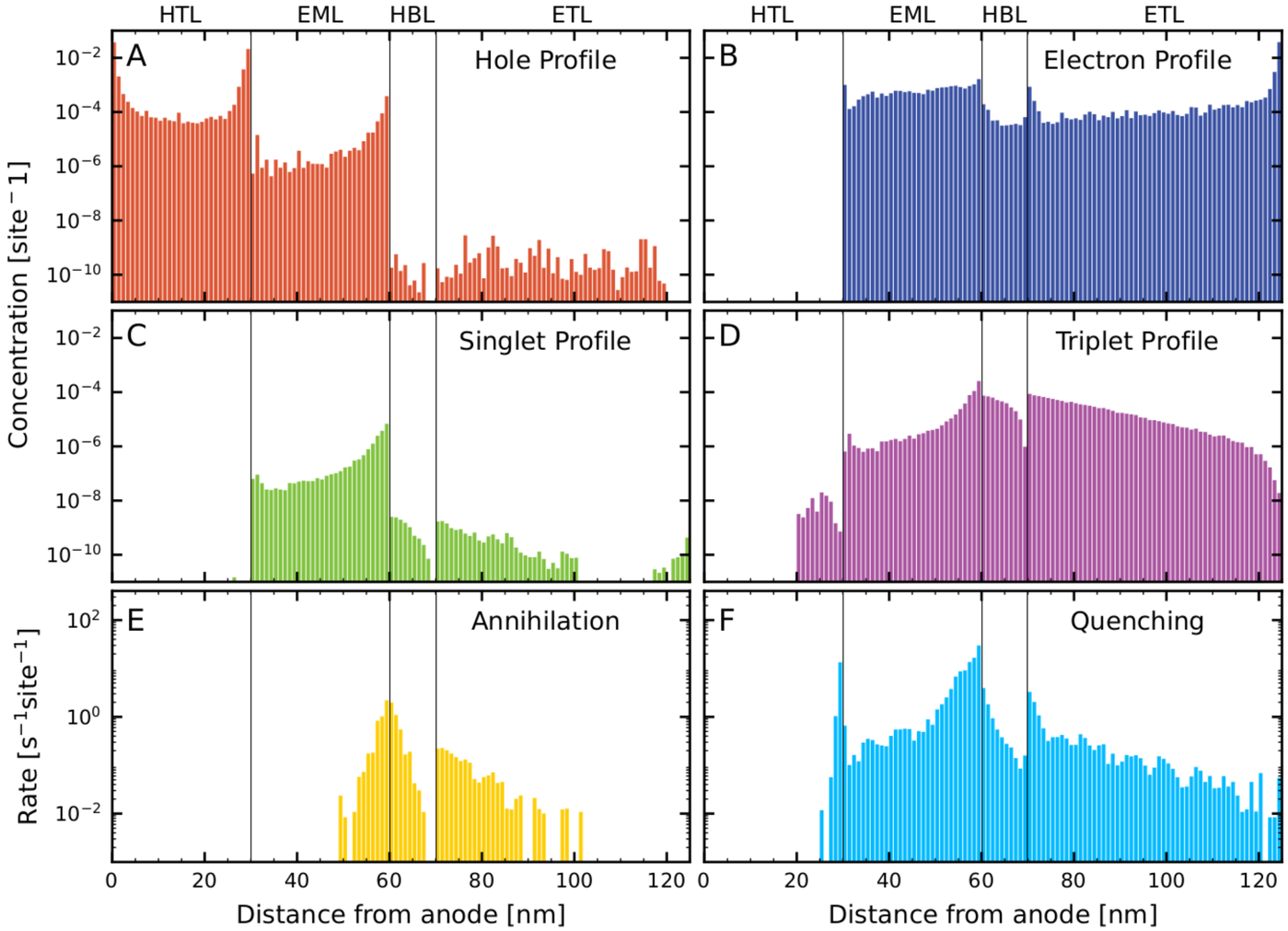


- Bulk-average Emission
- Focus on Optics

- Molecular Interactions
- Role of Morphology

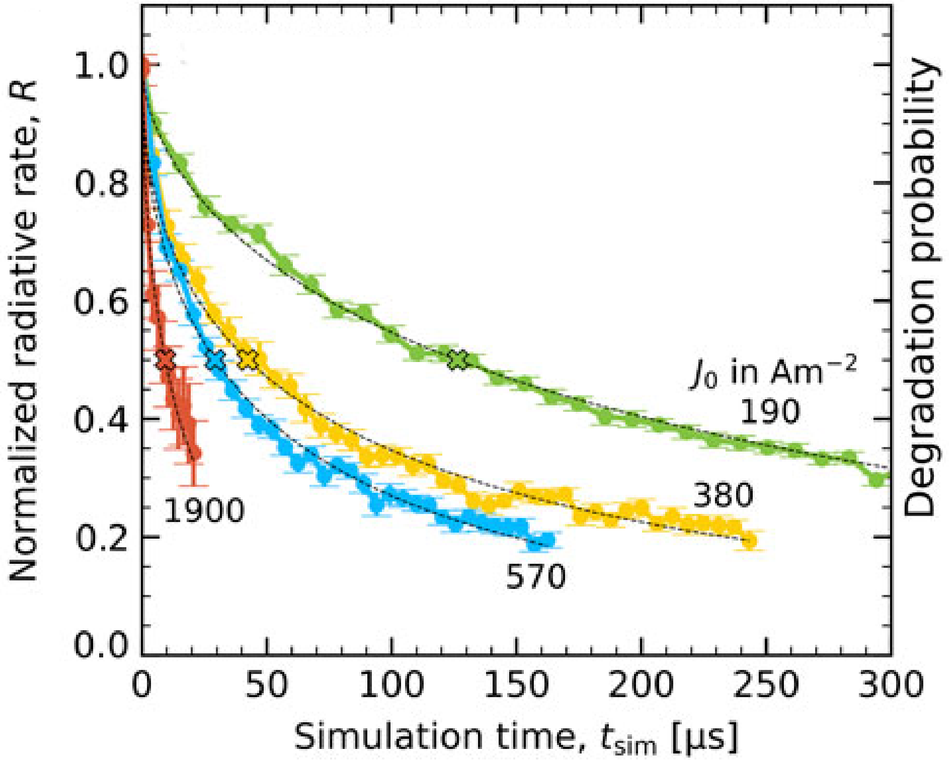
Nanoscale Analysis

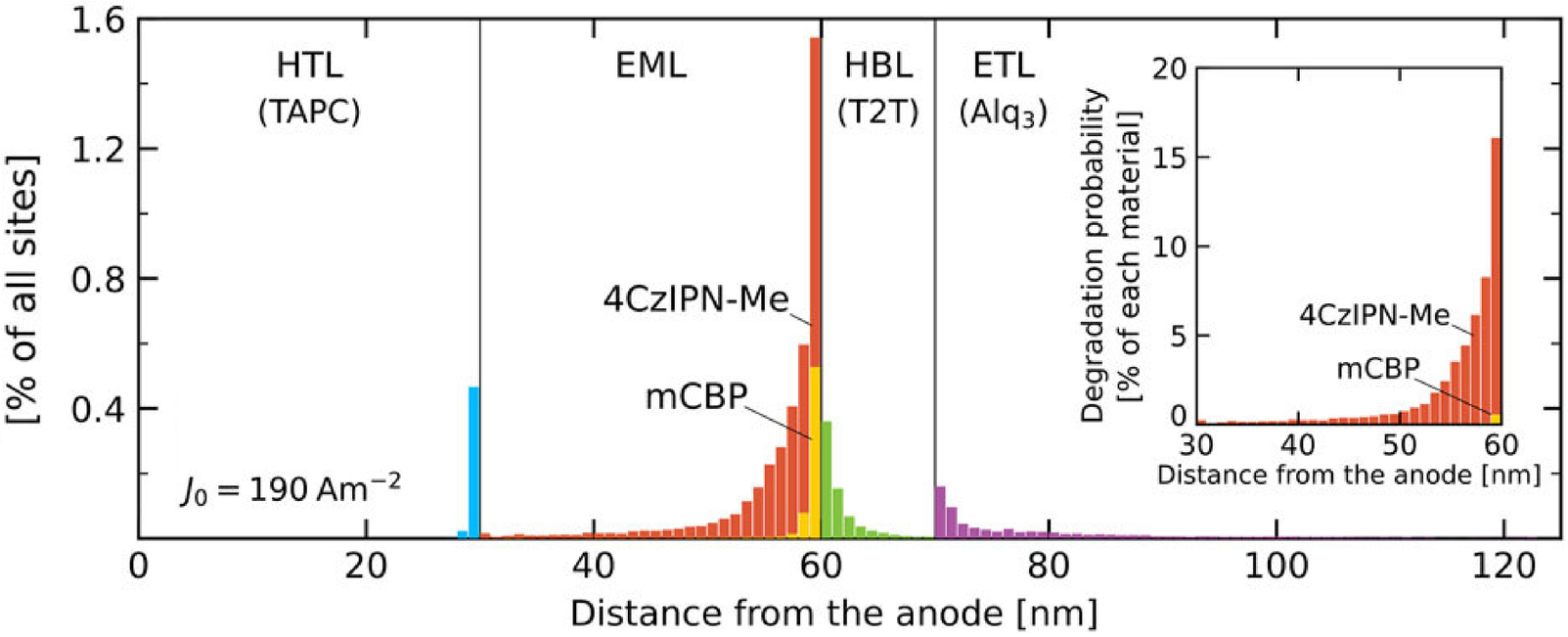




DOI: 10.3389/fchem.2021.823210

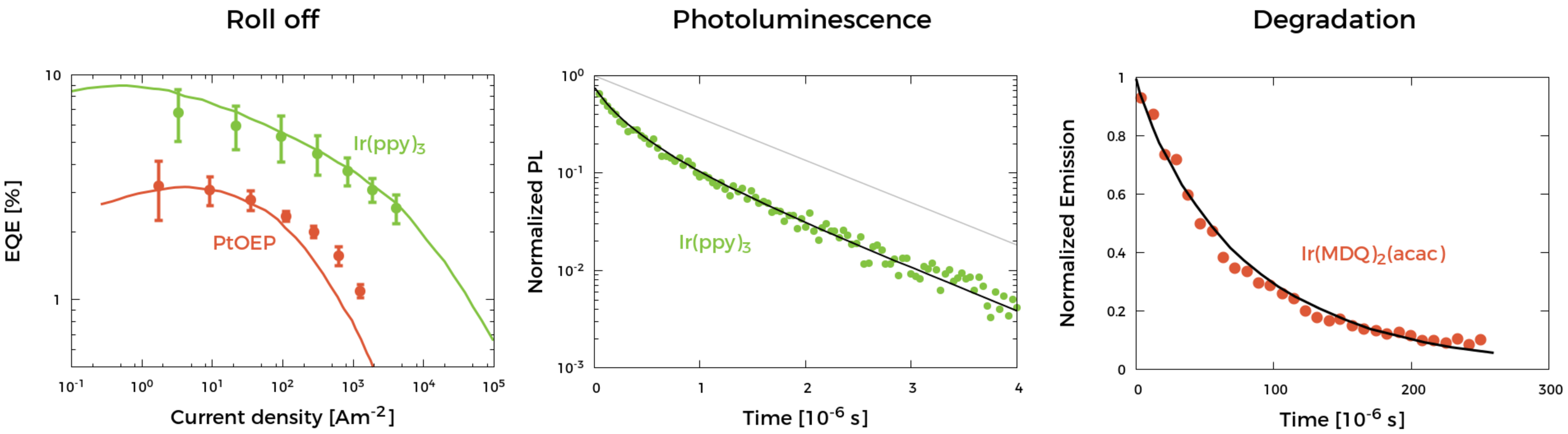
Lifetime Studies





DOI: 10.3389/fchem.2021.823210

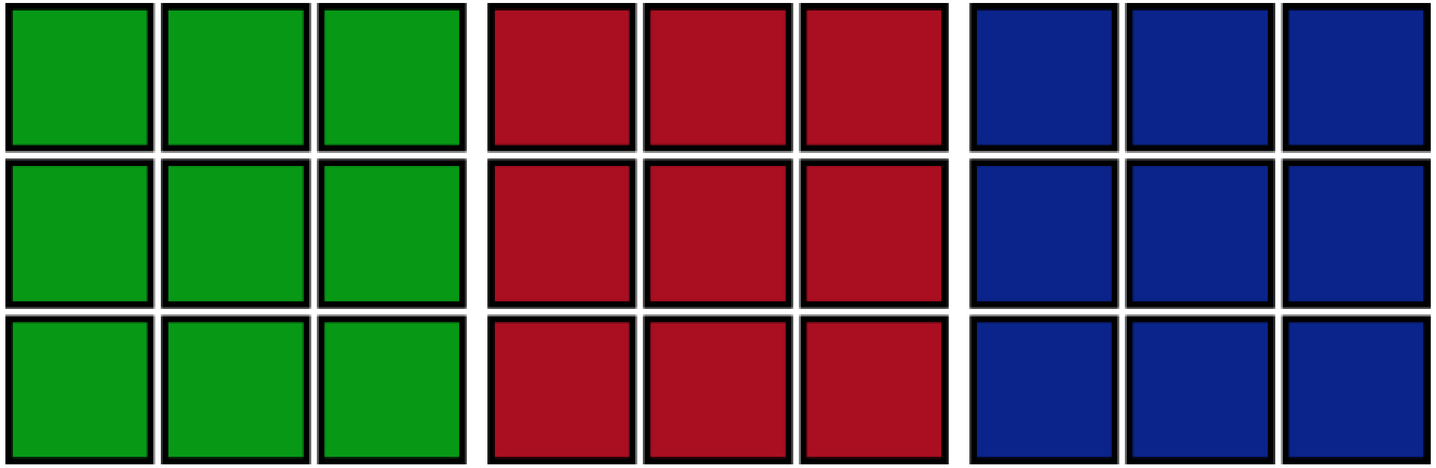
Device Efficiency

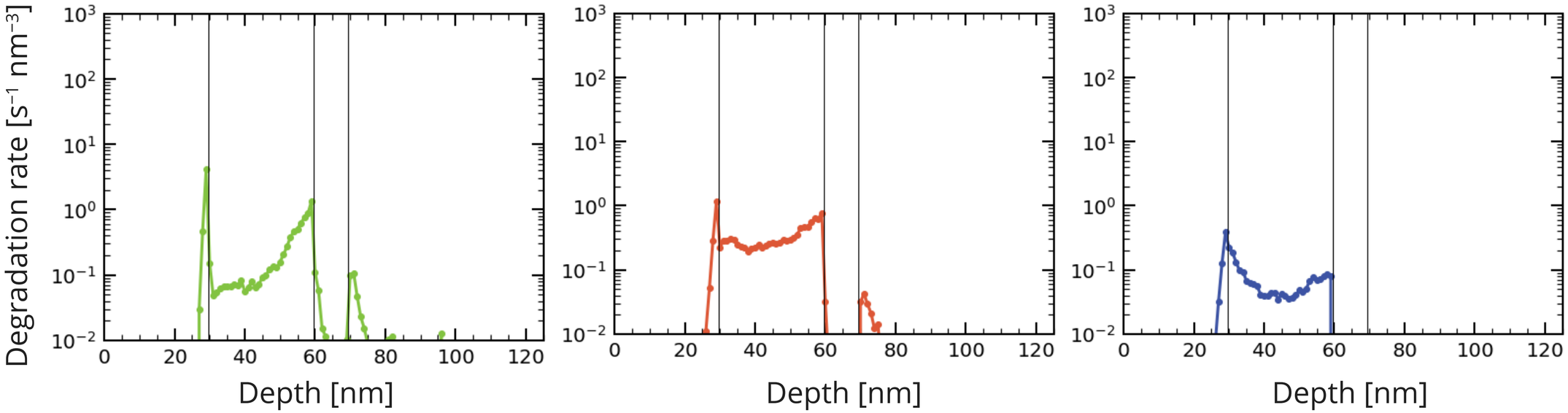


DOI: 10.1002/adfm.201402532

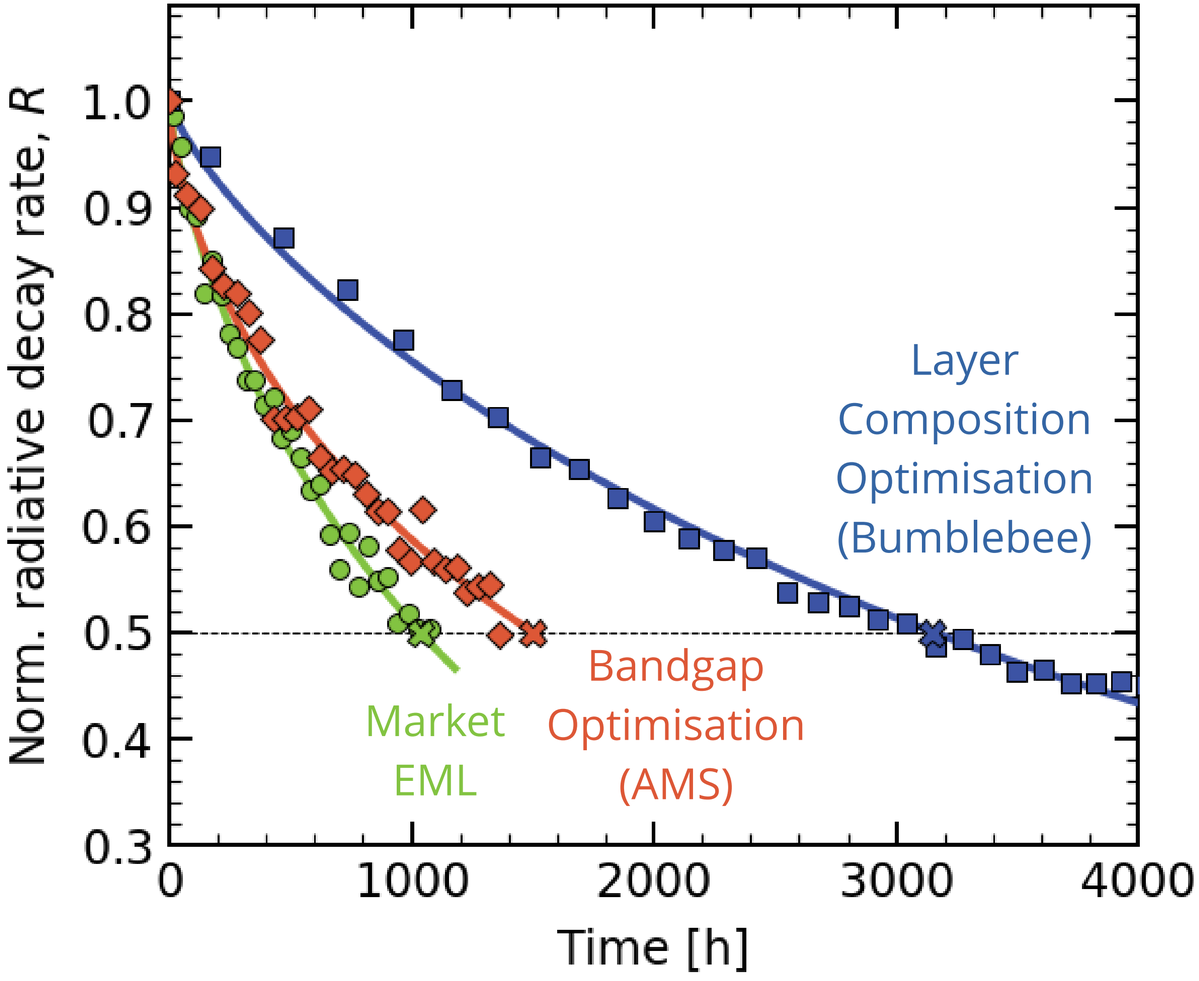
Pixel to Display

- Coarse-grained
- Pixel-to-pixel variance
- Colour stability



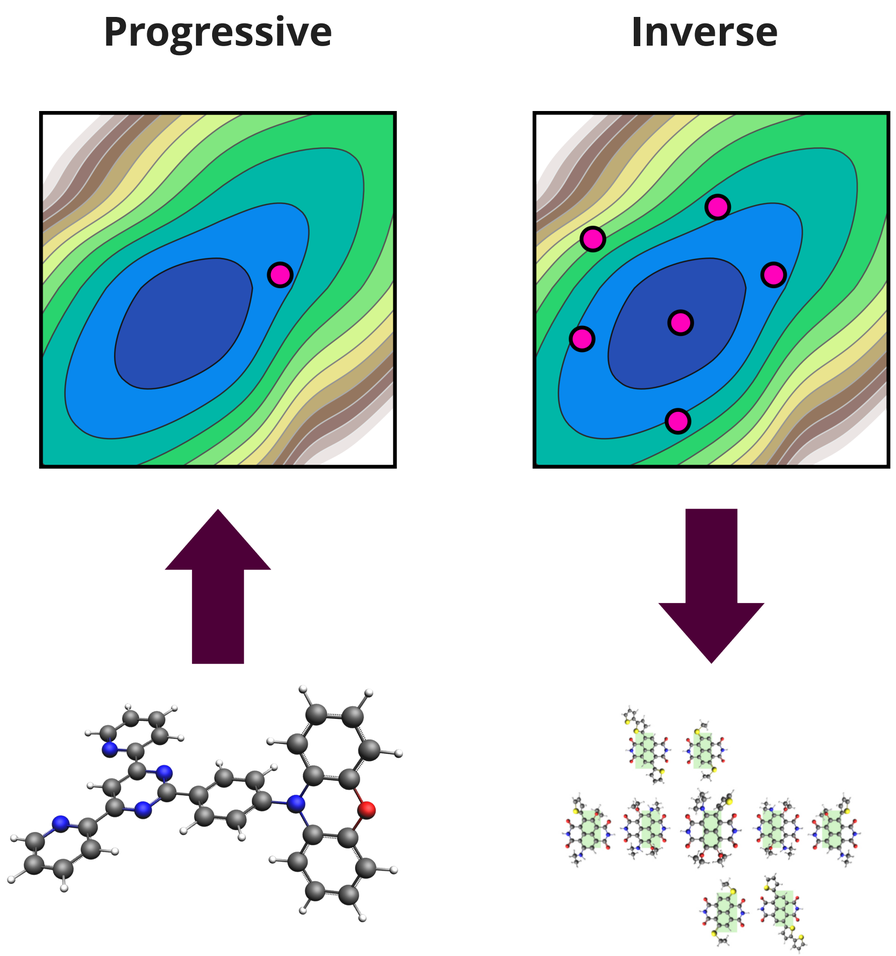


Integrated Design and Optimisation



Integrated Design and Optimisation

- 3D-kMC Stack Optimisation
  - Target Properties
- Molecular Screening with DFT, DFTB and COSMO
  - Ligand Optimisation
  - Compound Reaction Discovery
- Detailed atomistic refinement or experimental validation for high-value candidates



SCM
Software for Chemistry & Materials

Check out our Demo!

Bart Klumpers, klumpers@scm.com