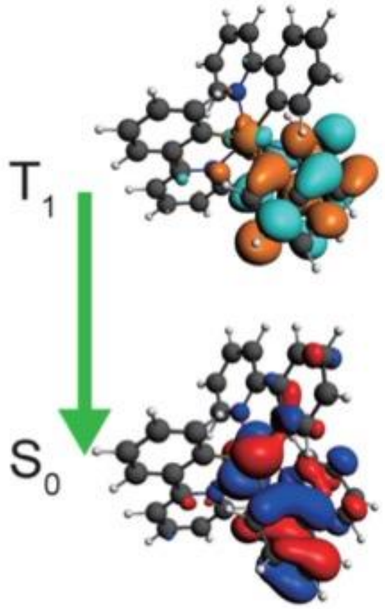
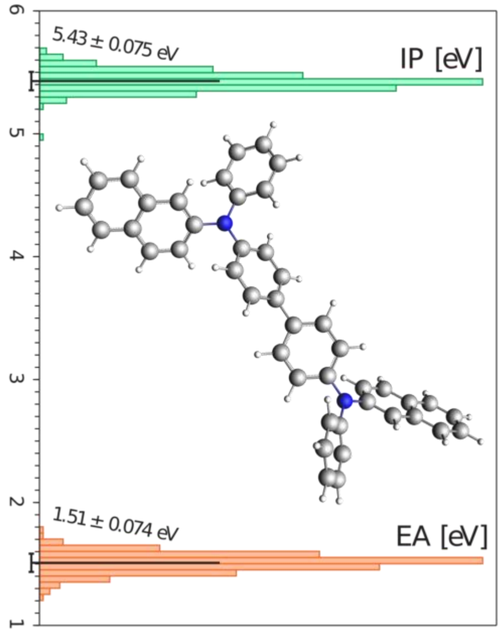
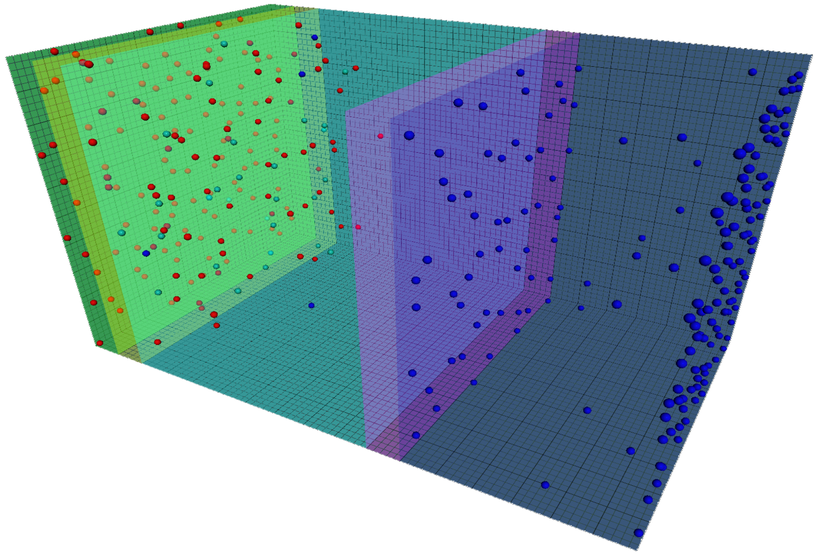
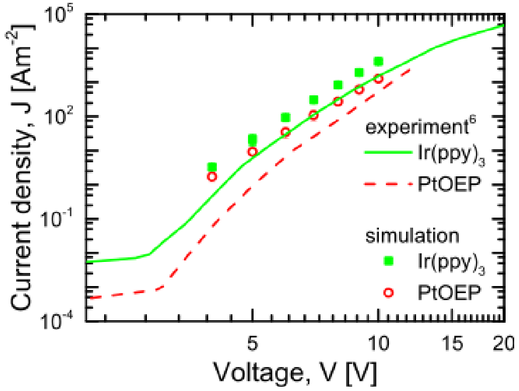
Accelerated OLED development

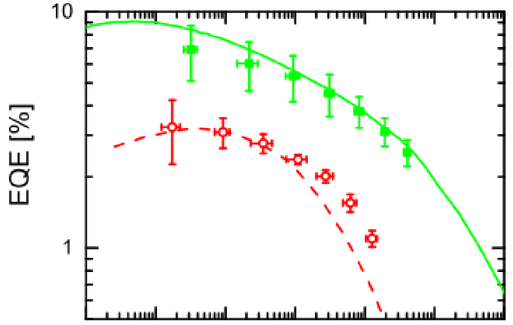
Through Multi-Scale Modeling











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Research Engineer, Simbeyond

SCM
Software for Chemistry & Materials

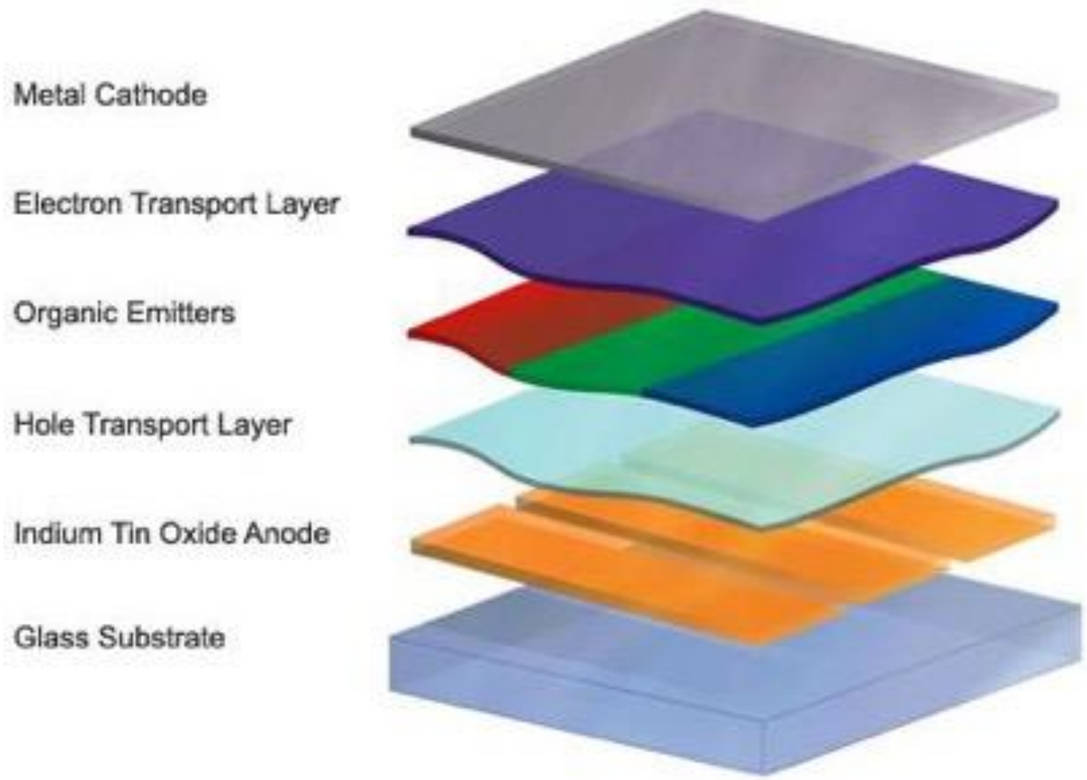
SIMBEYOND

New materials discovery too slow

- 8-19 years to develop materials solutions in new markets
- 80-85% R&D programs fail
- >50% R&D spending only incremental improvement
- Vicious circle: slow discovery ⇔ few new materials (expensive)
- Combining different materials in a device adds extra complexity

https://www.mckinsey.com/industries/chemicals/our-insights/chemical-innovation-an-investment-for-the-ages

Modeling: faster & cheaper new materials



- Maximize luminescence
- Optimize color
- Minimize destructive processes
- Optimize charge & exciton transport

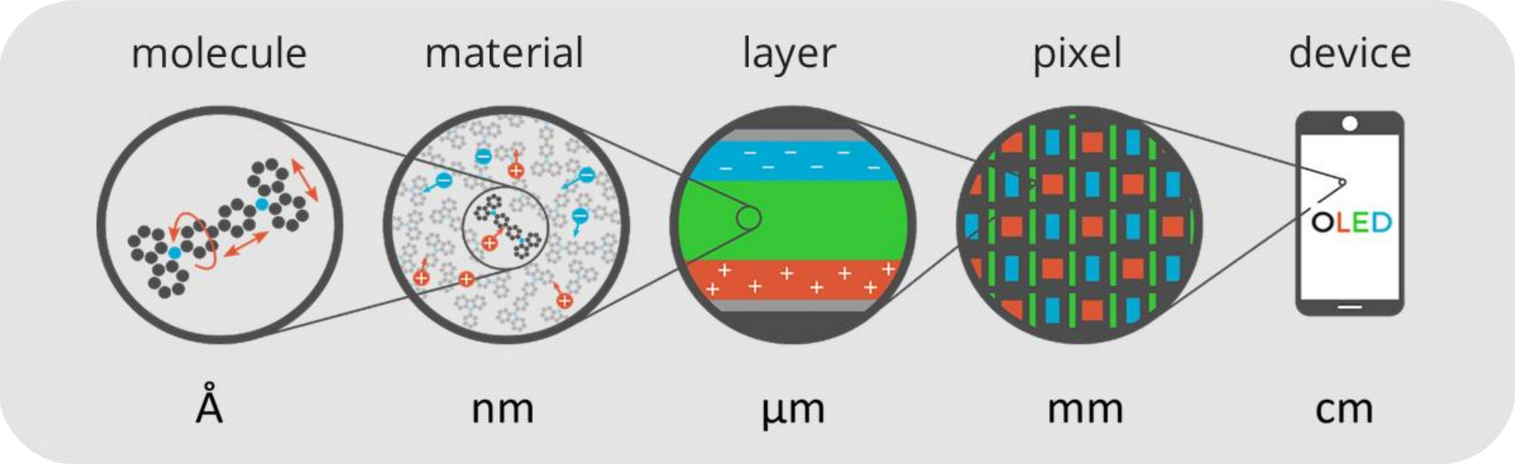
Atom & electrons determine single material properties

Predict, understand & improve with **atomistic modeling**

Interactions between materials determine device-level behavior

Predict, understand & improve with **meso- & macroscale modeling**

Collaboration between Simbeyond & SCM



SCM

Calculating molecular level properties such as:

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

of each molecule in a realistic morphology

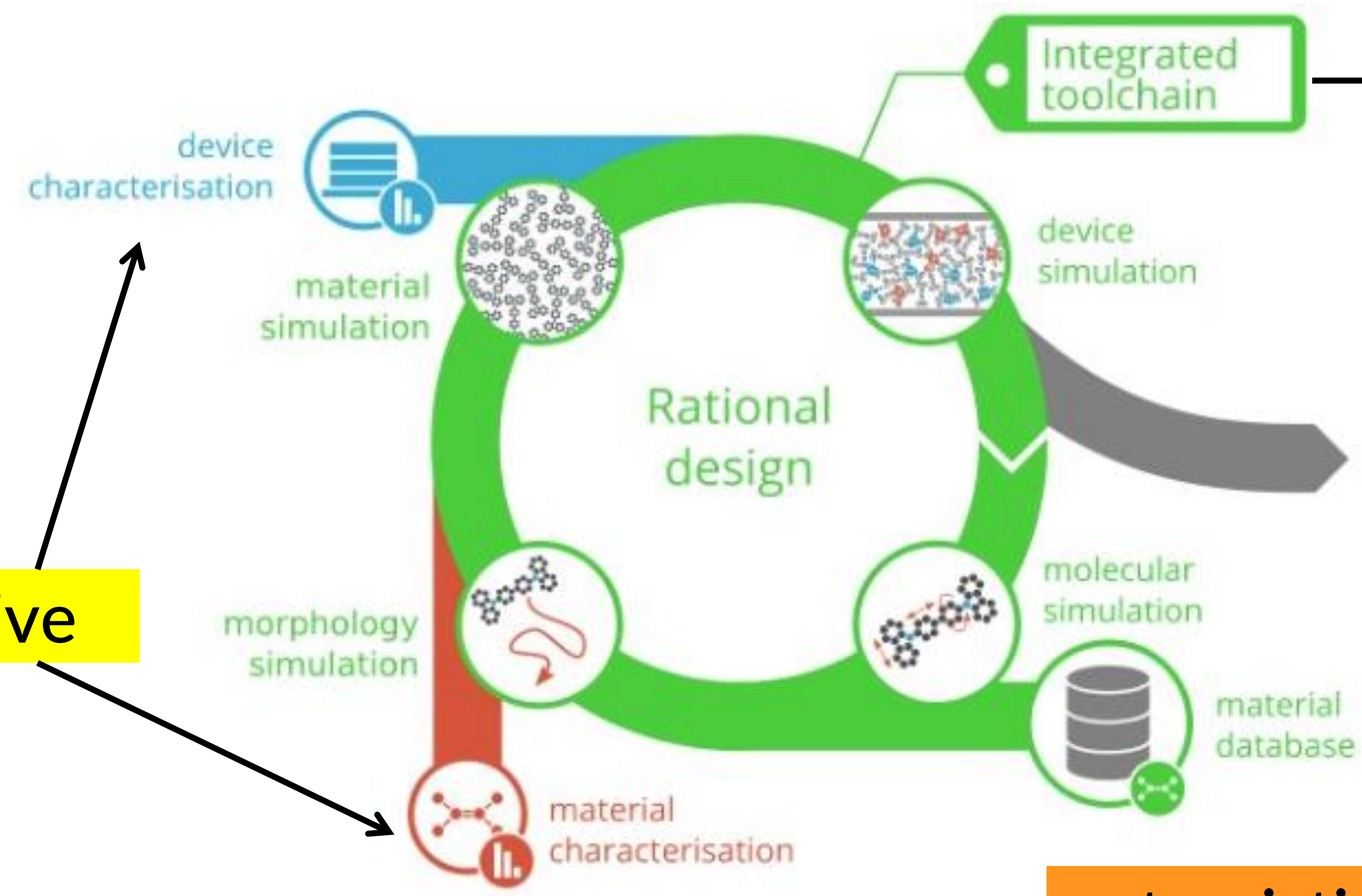
SIMBEYOND

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

OLEDs: Optimize many materials & properties



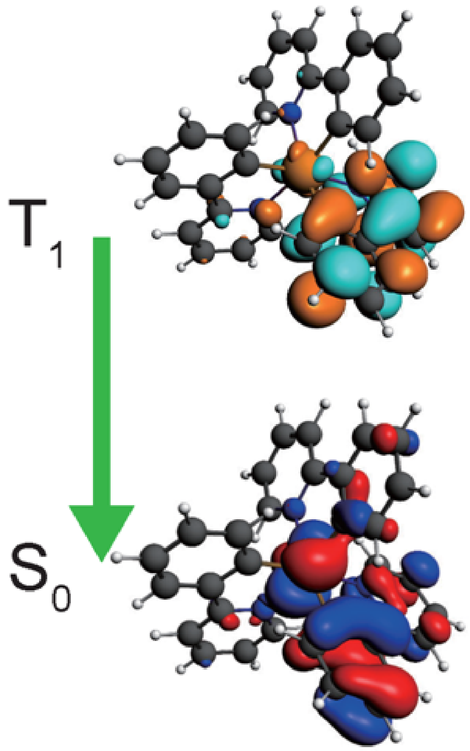
Predict promising materials + stacks

Expensive

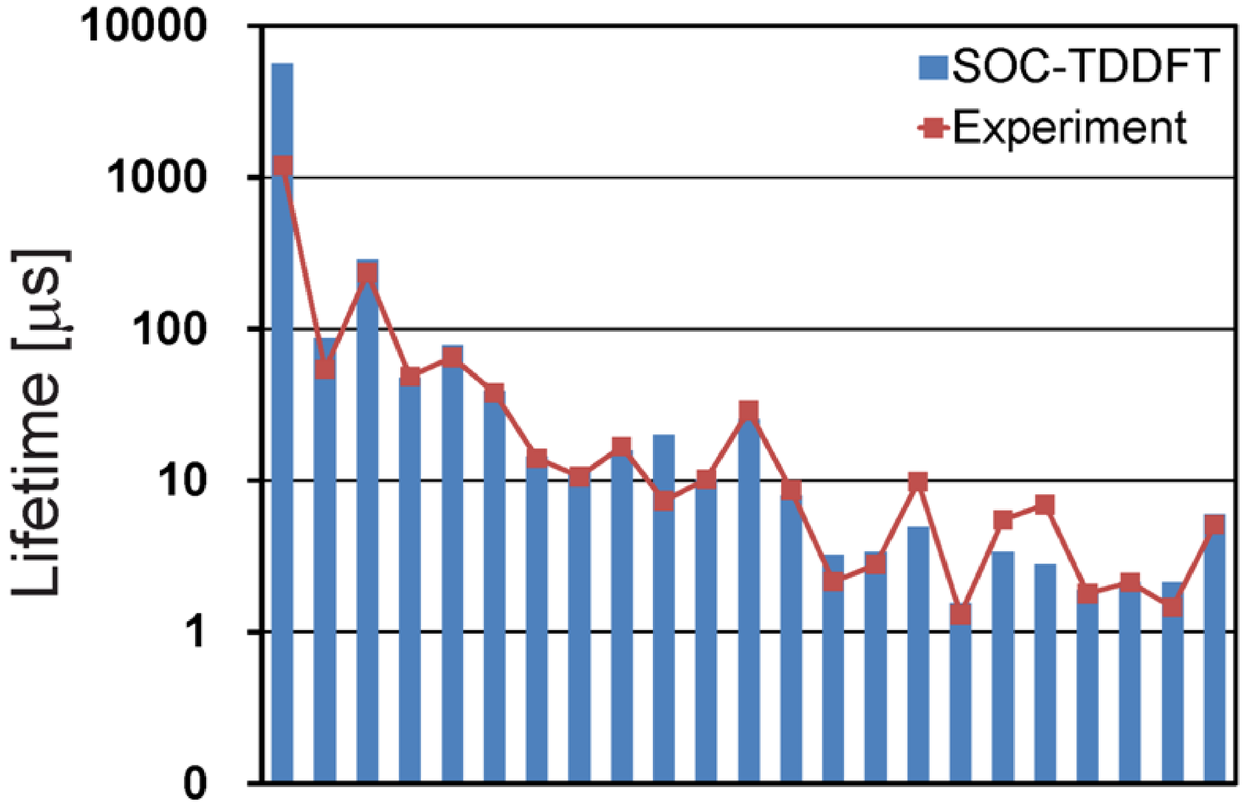
Simulation
Material experiments
Device experiments
New product

atomistic + device-level simulations:
focus on the best materials + stacks
reduce costs & time to market

Optimize OLED emitter lifetimes



Phosphorescence



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

ADF: Spin-orbit TDDFT [phosphorescence lifetimes]

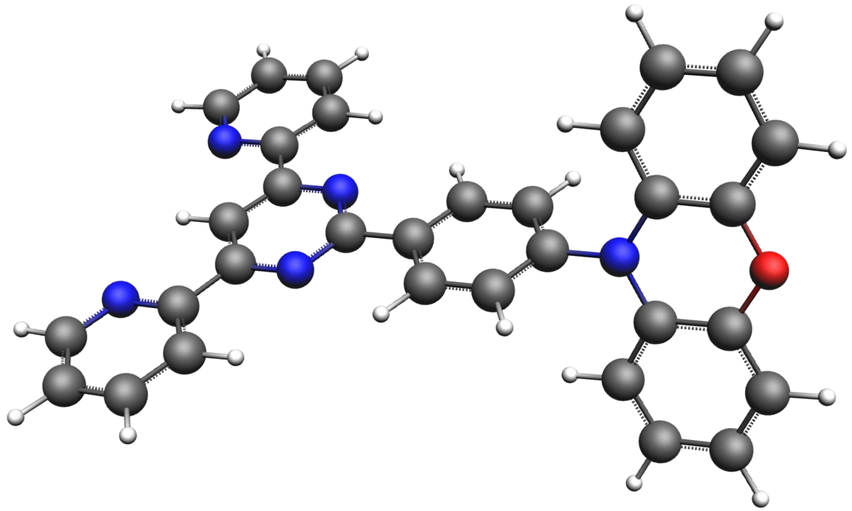
[PCCP 16, 14523 (2014)]

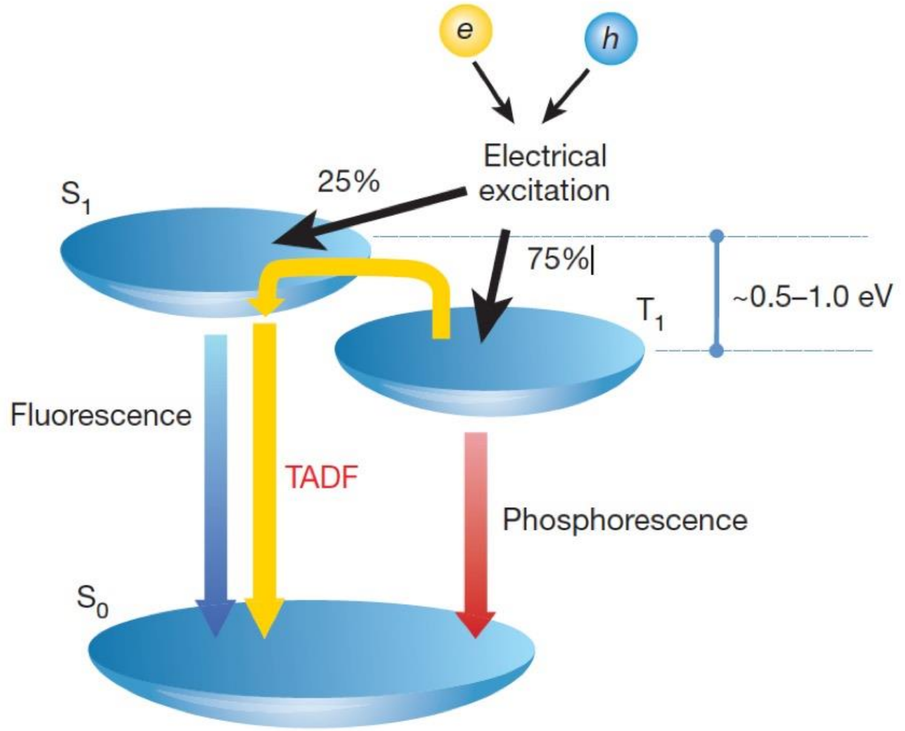
- **BASF**: efficient blue emitter ([Adv. Mater. 2010]), [patent 2016] (=> UDC)
- **DuPont**: protocol for screening lifetimes ([JPCC 2013])

Optimize TADF emitters

Spin-orbit TDDFT => Intersystem crossing

- Minimize S_1-T_1 gap
- Maximize SOC
- Maximize k_{phos} & k_{TADF}

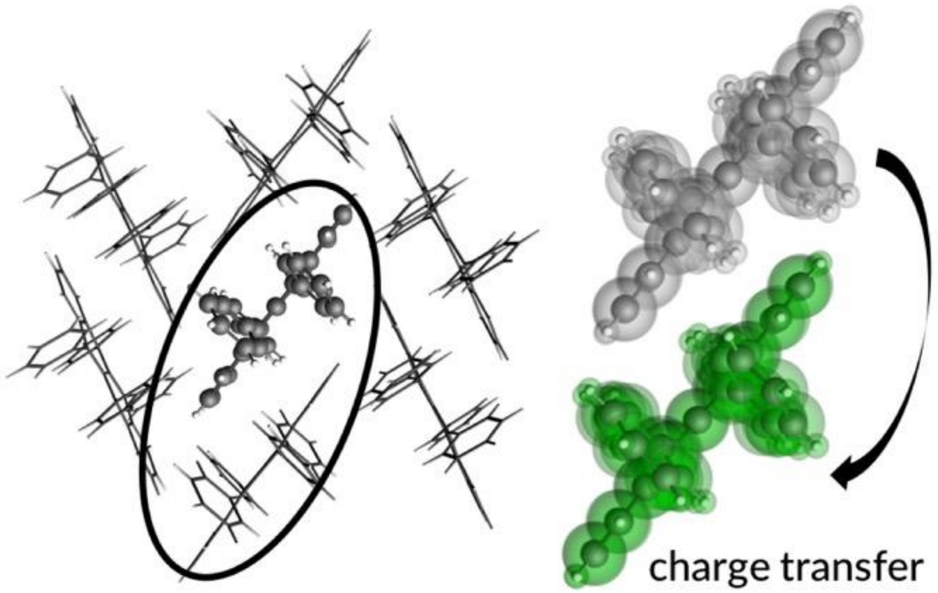


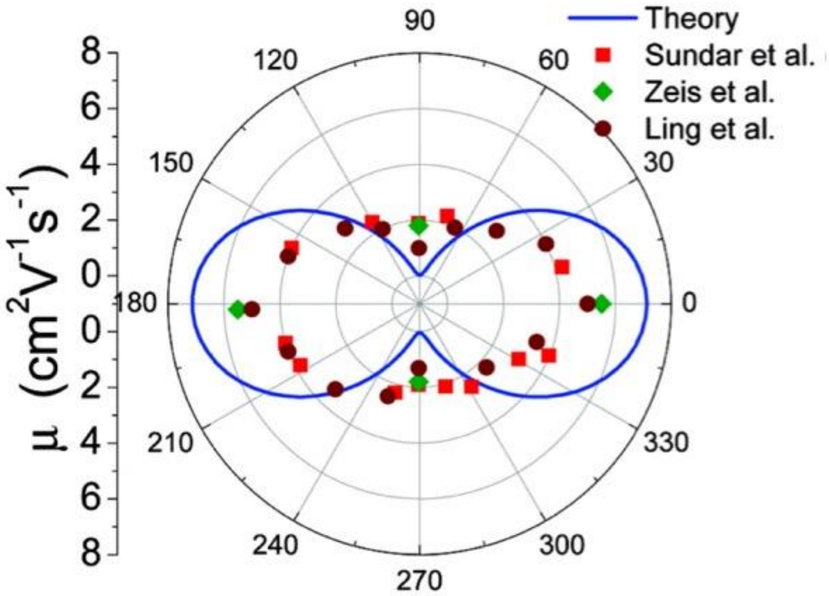


- Z.-M. Su et al Dyes & Pigments 2017, Bredas et al. J. Am. Chem. Soc. 2017
- **OSRAM**: patent 2018
- **Cynora**: patent 2019
- **Samsung**: blue TADF emitter, Nanomat. 2019; Organic Electronics 2020

Optimize charge mobility

- J. Chem. Phys. 2007: organic semiconductors (**BASF**): hole and electron mobility



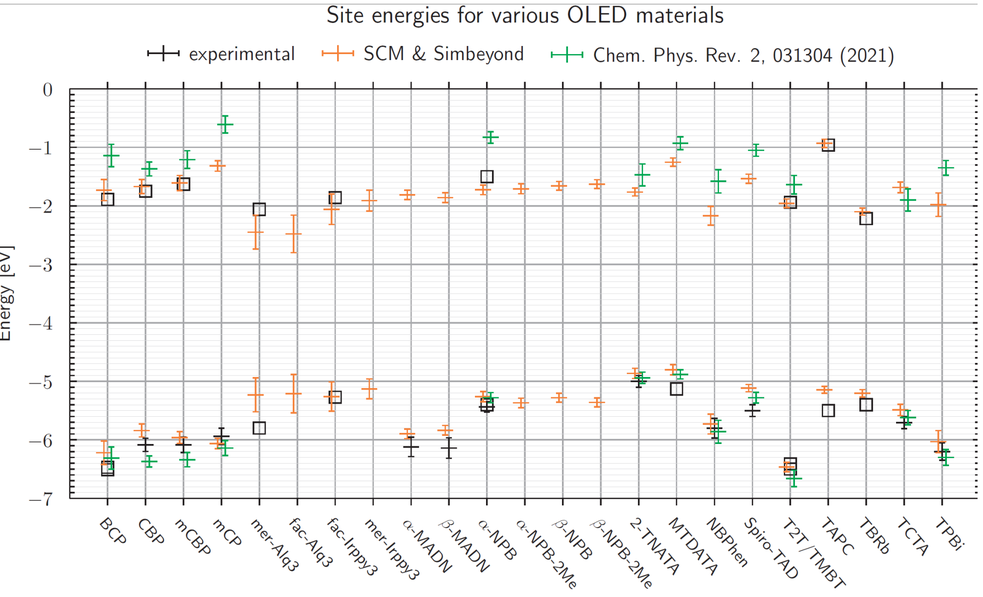


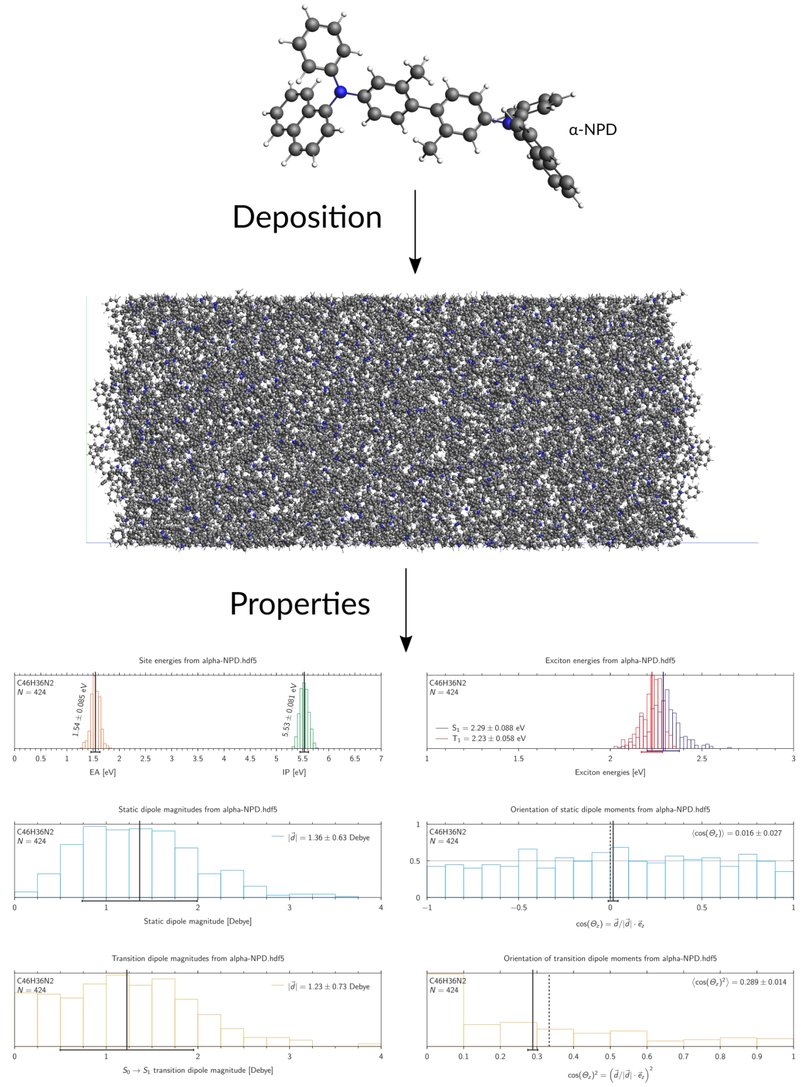
- many patents (2015-now)
- Solubility / miscibility: COSMO-RS

Related:

- Charge generation
- Charge recombination
- Exciton transfer

Ionization Potentials & Electron Affinities: workflow





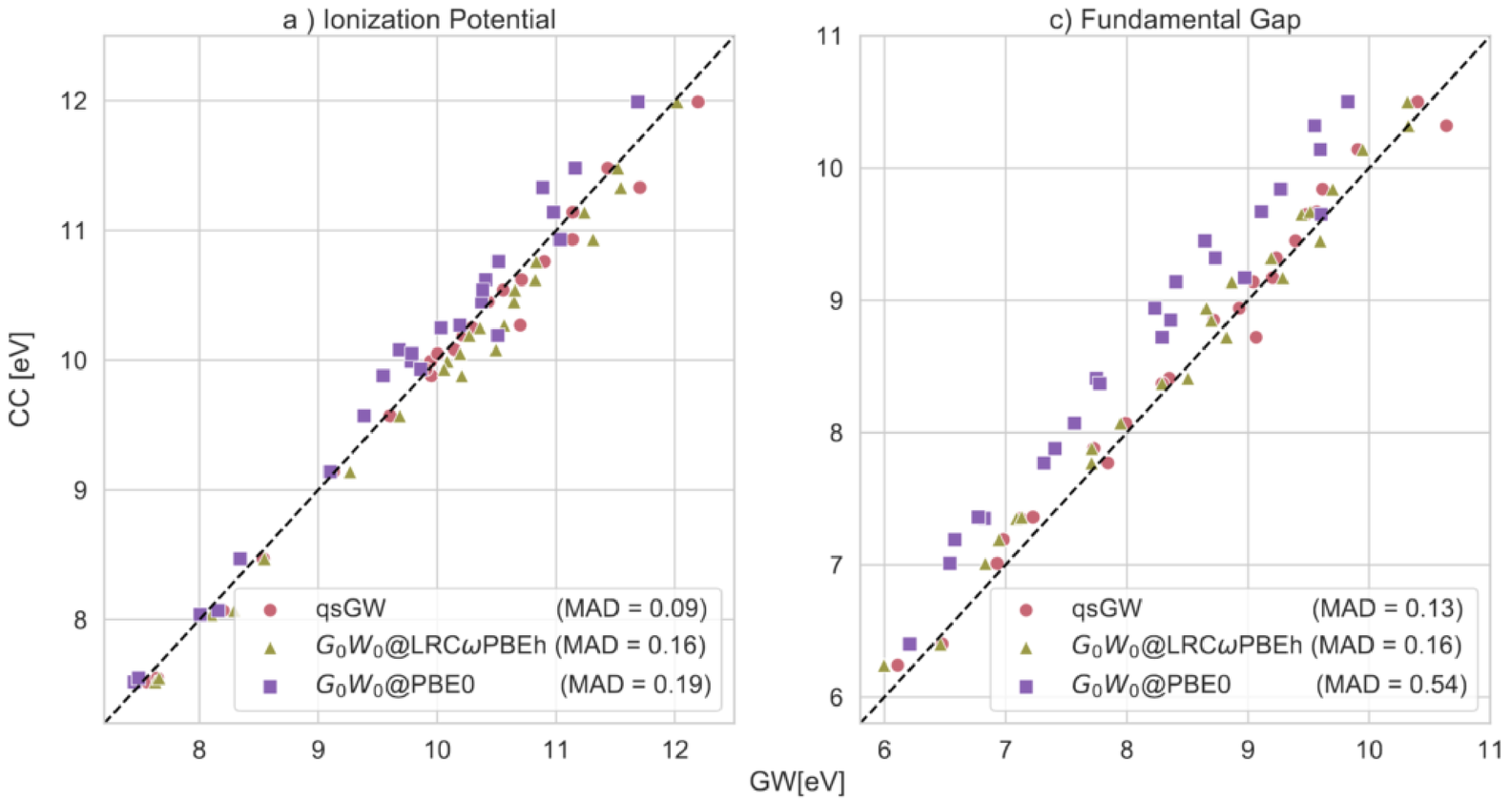
1) deposit (UFF4MOF-II)
- fbMC
- Use graphite support
- Fix bottom layers
- Remove support

Video

2) Opt neutral, cation, anion
- xTB/UFF4MOF-II

3) Calculate properties
- IP, EA: DFT+embedding
- Transfer integrals
- Exciton properties

Ionization Potentials & Electron Affinities: qsGW



- Quasiparticle self-consistent: works with GGA
- DABNA-1 with TZ3P basis: 3.5h@32 cores

- AMS2023:
- Spin-orbit coupling
- qsGW-BSE: excitations

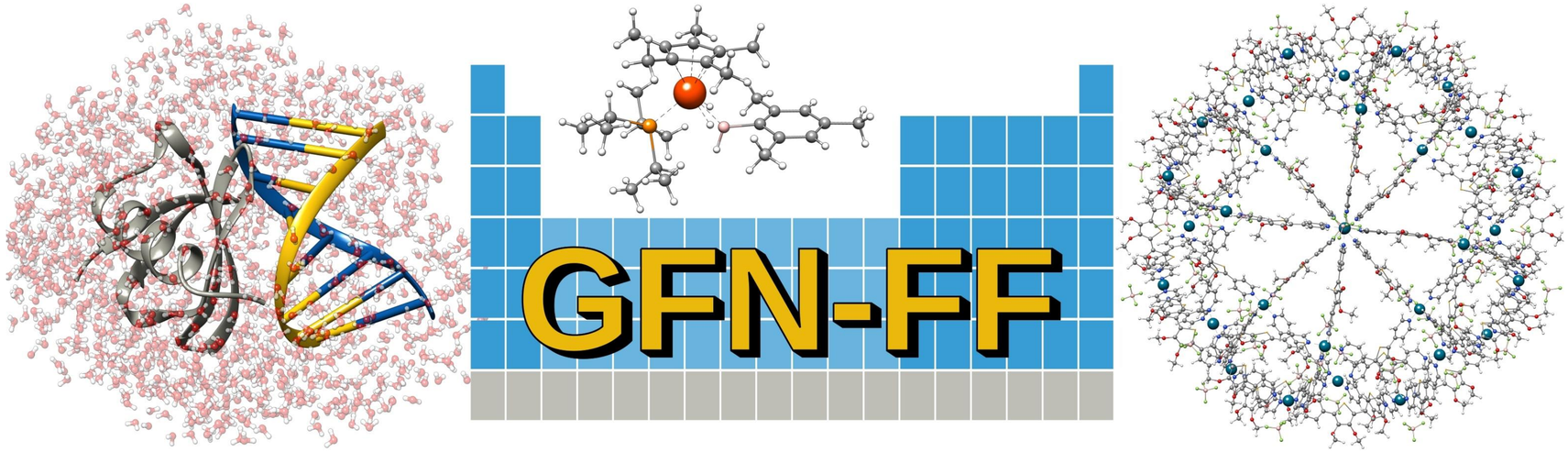
- To do: qsGW + environment

Option: qsGW + DFT environment

Förster A. and Visscher L. (2021) Low-Order Scaling Quasiparticle Self-Consistent GW for Molecules. Front. Chem. 9:736591 (2021)

GFN-FF

- Automatic, general, partially polarizable force field
  - Covalent + non-bonded terms, some extended Huckel
  - Quadratic scaling
  - Organometallics, MOFs, biochemicals
  - Molecule or bulk

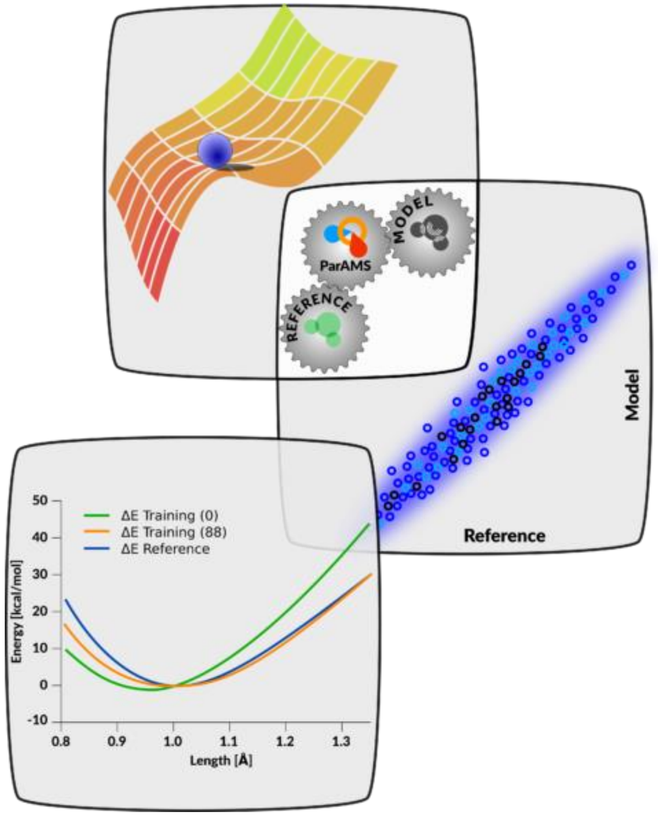


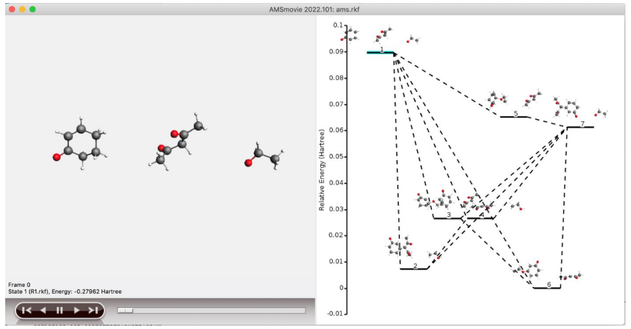
S. Spicher, S. Grimme. *Robust Atomistic Modeling of Materials, Organometallic, and Biochemical Systems*, Angew. Chemie Int. Edit. 59, 15665-15673 (2020)

New in AMS2022:
Parametrization, auto reaction pathways

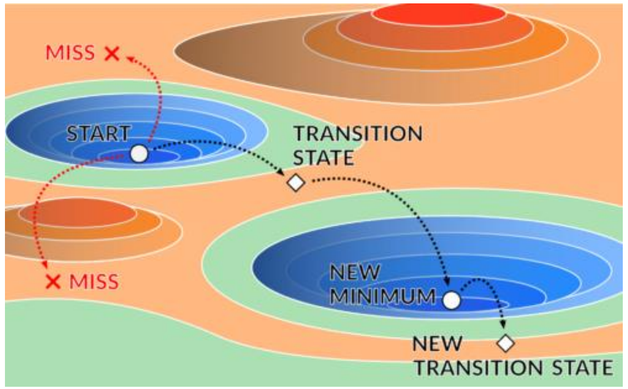
- Build training sets with AMS
- Define cost function
- Optimize parameters
  - Lennard-Jones
  - ReaxFF
  - DFTB
  - Future: GFN-FF, ML Potentials, … ?

ParAMS





- EON + ACE Reaction (Auto TS search)
- Find reaction networks, minima, TSs
- Refinement of TSs with higher-level
- Determine and visualize binding sites
- ChemTraYzer2: reaction rates + fluxes
- kMC (interface to Zacros)
- 2023: m3gnet – universal ML potentials



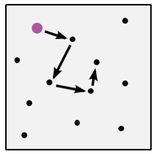
Processes relevant for device

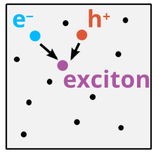
- Electronic
  - Charge injection, hopping, collection
  - Coulomb, external fields, image potential

- Excitonic processes
  - Diffusion
  - Generation, dissociation
  - Annihilation, polaron quenching
  - Non-radiative decay

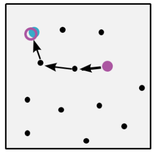
- Degradation processes

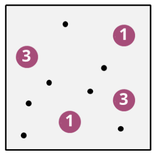
kMC with experimental or **computed rates**
Integrated atomistic to device


Exciton diffusion:
– Förster
– Dexter

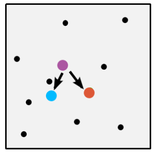


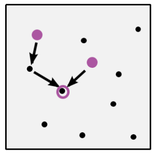
Exciton generation

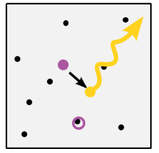

Exciton-polaron quenching



(Reverse) Inter-system crossing

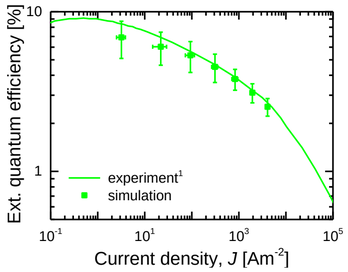

Exciton dissociation


Exciton-exciton annihilation

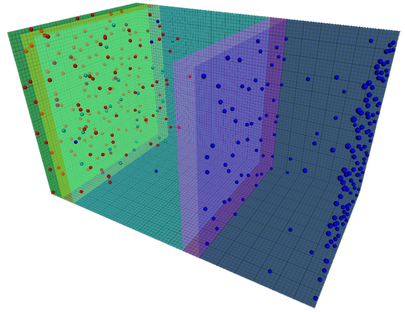

(Non-)radiative decay

Device-level predictions & insights

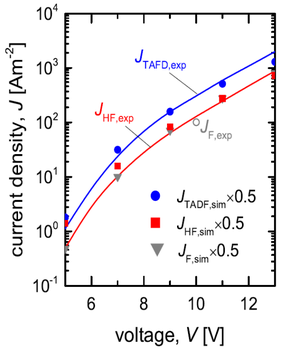
Efficiency roll-off



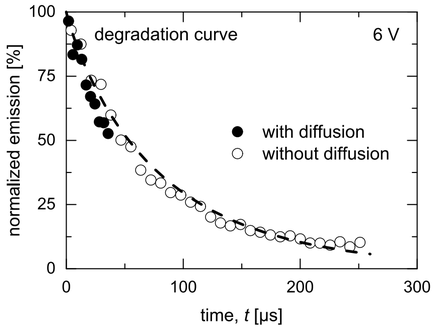
3D visualization



J(*V*) characteristics

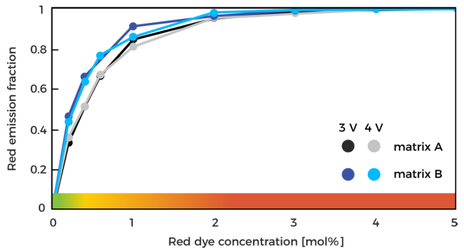


Device lifetime

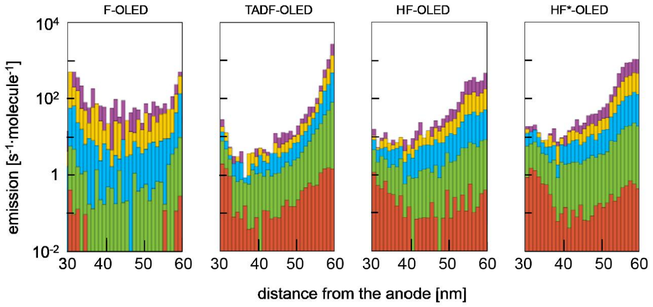


bumblebee™

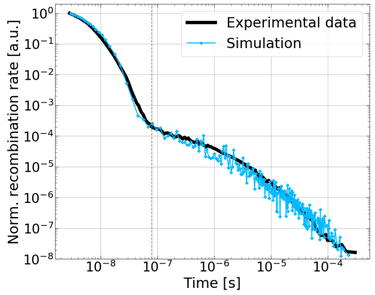
Color point shifts



Profiles



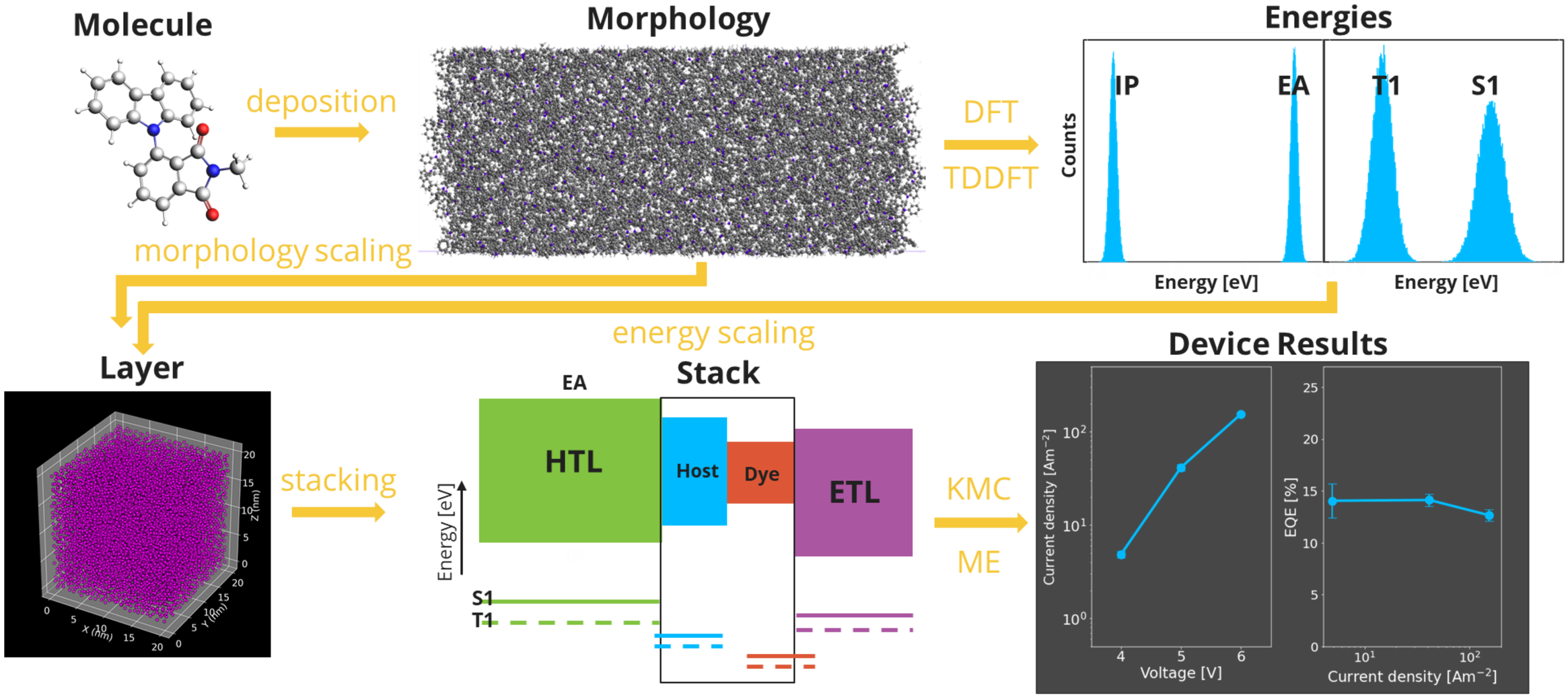
Transient behavior



Nature Mater. **12**, 652 (2013)
Appl. Phys. Lett. **105**, 143303 (2014)
Adv. Funct. Mater. **25**, 2024–2037 (2015)
Appl. Phys. Lett. **114**, 073301 (2019)

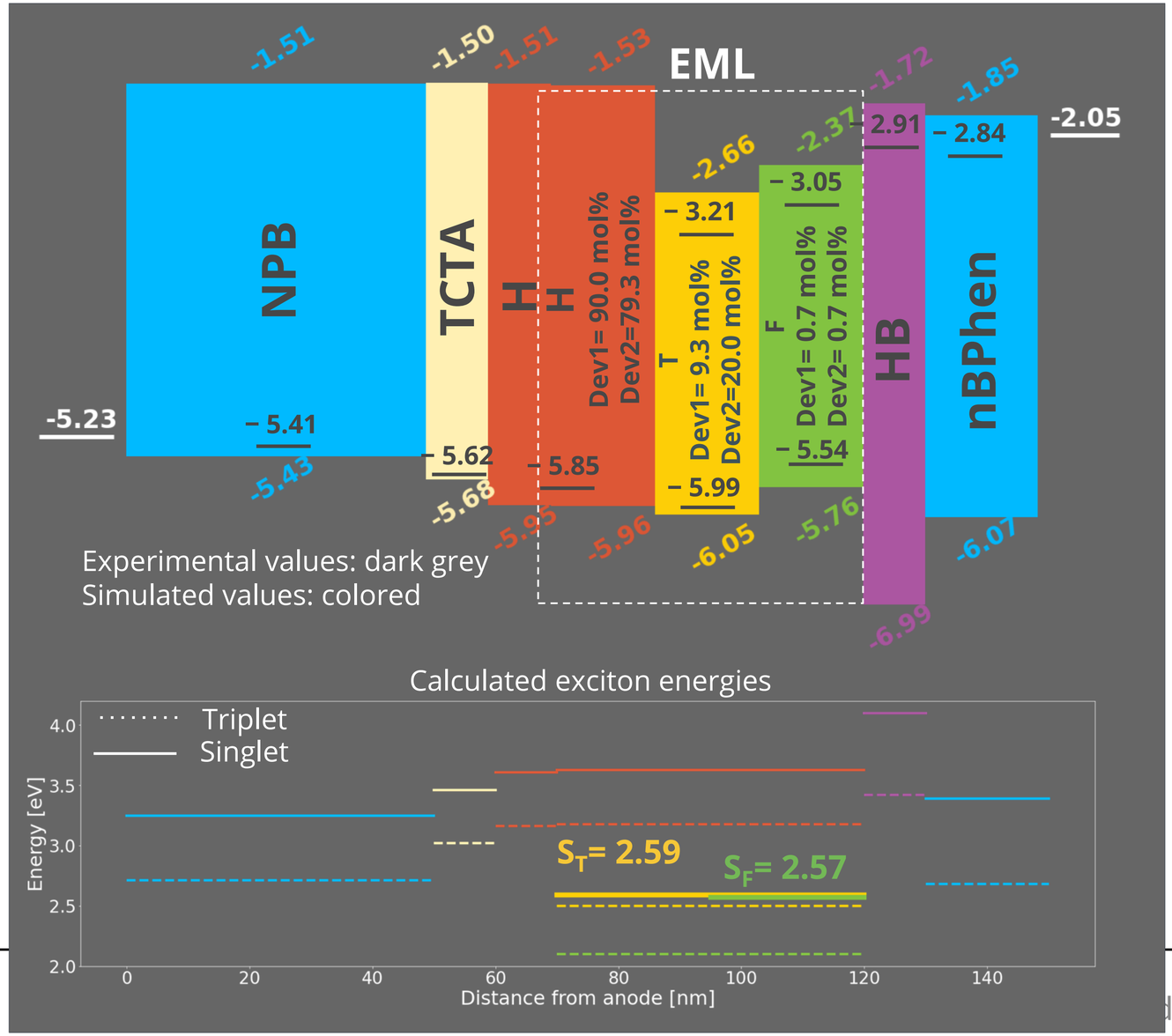
Experimental results from
Phys. Rev. B **77**, 235215 (2008)
J. Phys. Chem. C **121,** 8515 (2017)
Sci. Rep. **5**, 8429 (2015)

Multiscale toolchain: overall workflow

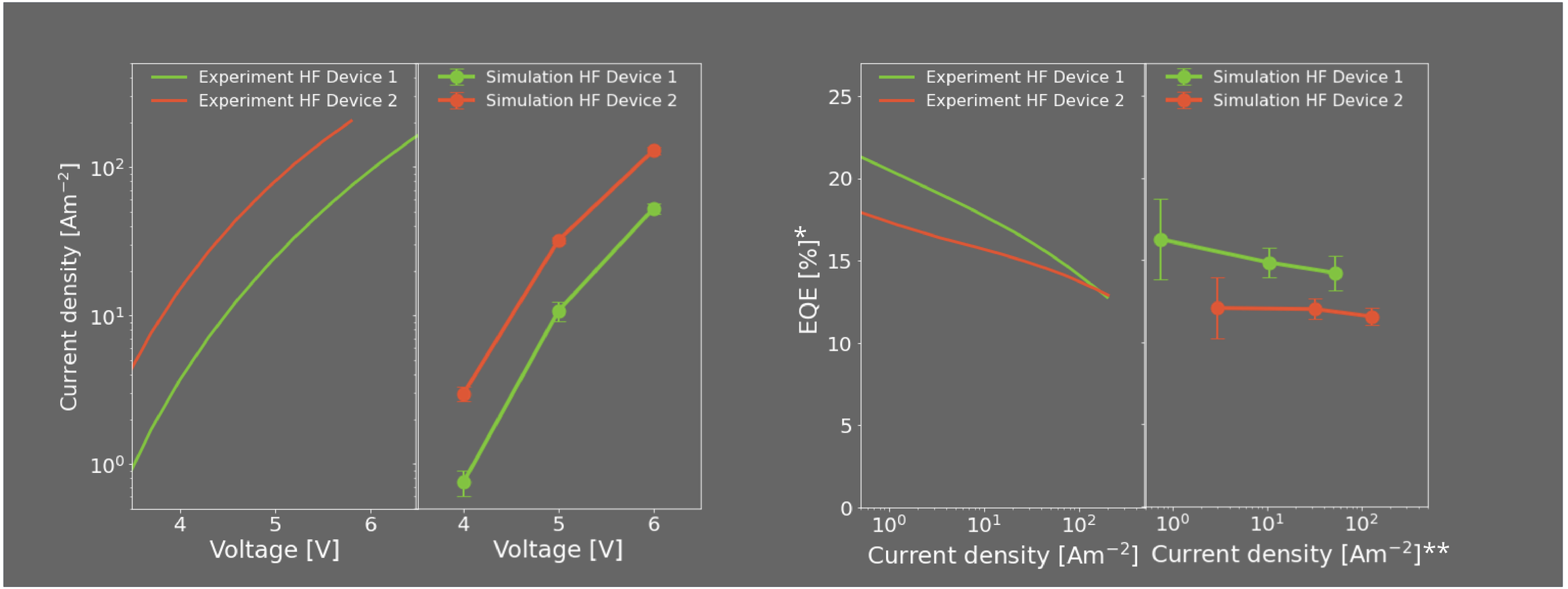


Molecular scale predictions Cynora HF stacks

- **IP (HOMO) values**: reasonably good agreement between predicted and experimental results
- **EA (LUMO) values**: differences between calculated and experimental results can be understood in the context of an inconsistent consideration of the exciton binding energy in conventional EA experiments.
- **Excitonic energies**: reasonably good agreement between predicted (2.59 eV) and experimental (2.65 eV) singlet energy of T molecule and predicted (2.57 eV) and experimental (2.45 eV) singlet energy of F molecules.
- **Ordering** of the exciton energies are as expected



Device level predictions Cynora HF stacks



- The experimental trend in the J(V) is very well predicted
- The experimental trend in the EQE is reasonably well predicted

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