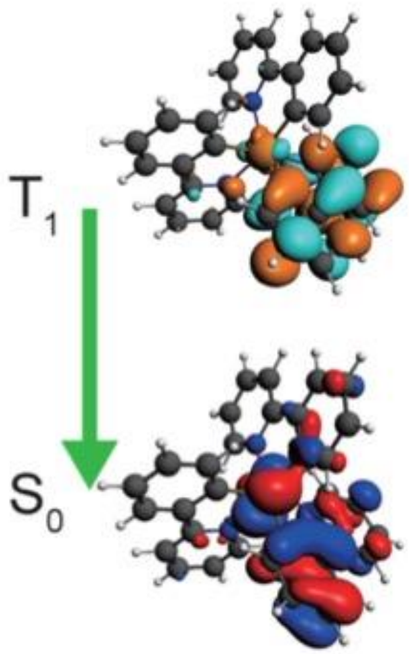
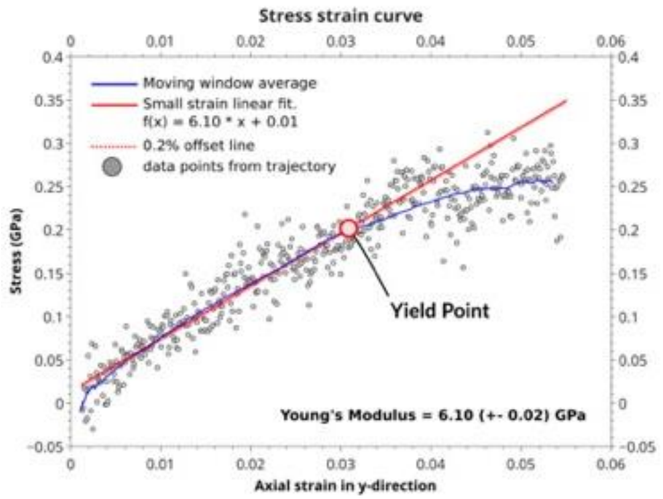
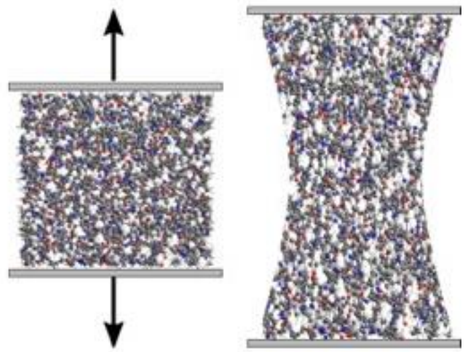
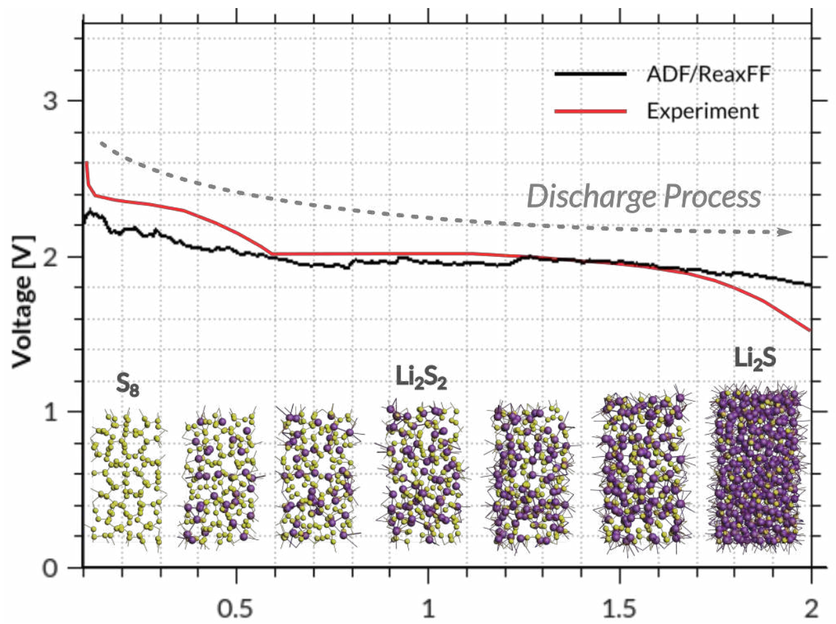
Accelerated Materials Discovery:
OLEDs, catalysts, polymers, batteries

Reducing time to market & research costs
through computer-aided design and multi-scale modeling







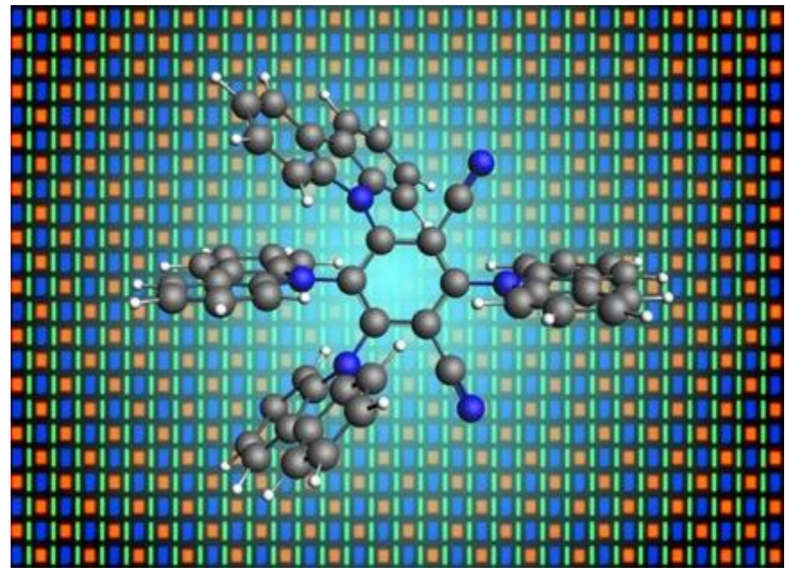


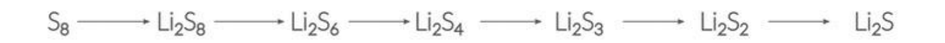
Fedor Goumans, Chief Customer Officer

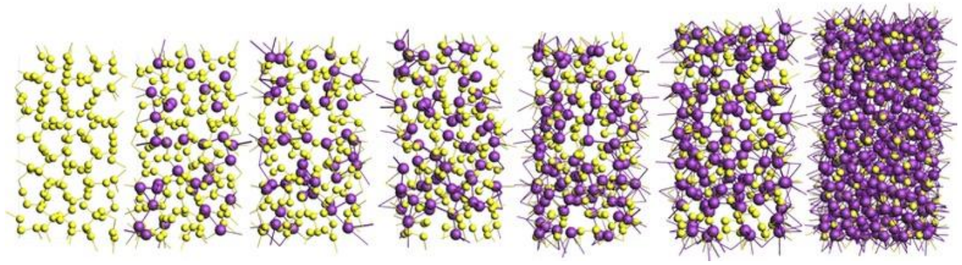
goumans@scm.com

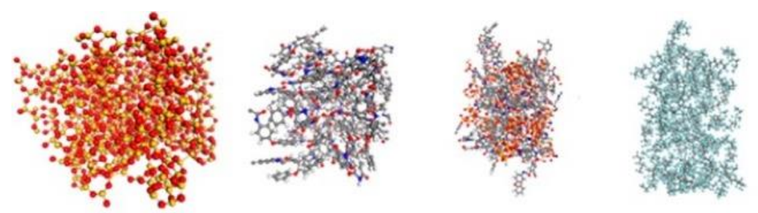
Contents

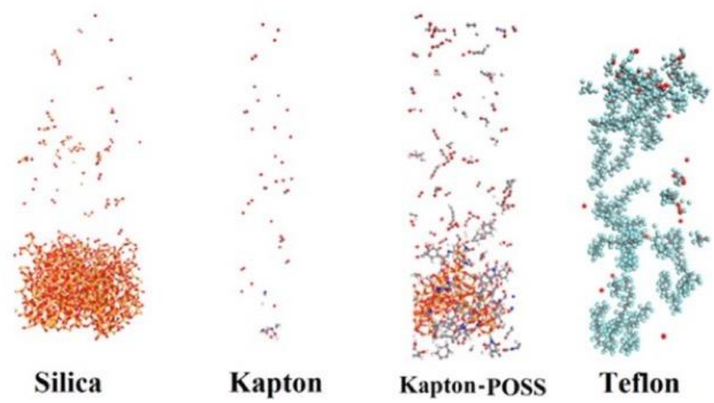
- History & overview
  - Background, Software Products
  - Collaborative projects
- Current capabilities
  - Catalysts
  - Display materials, OLEDs
  - Batteries
  - Polymers
- Multi-scale developments
  - Multi-scale reactor modeling
  - Multi-scale device modeling: OLEDs, batteries











Software for Chemistry & Materials

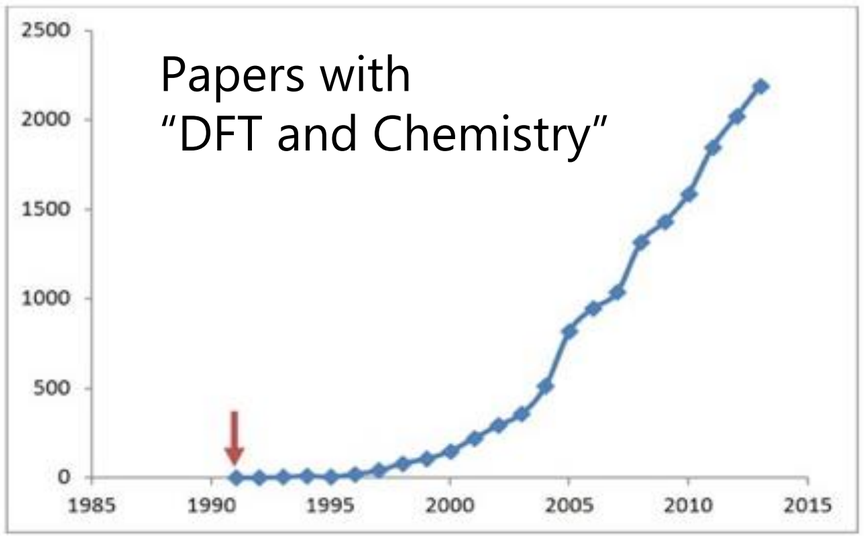
- SCM: Spin-off company from VU (1995)
  - Develop & market Amsterdam Density Functional (ADF)
  - Continued development: Amsterdam Modeling Suite

- ADF = first DFT code for chemistry (1970s)
  Baerends@VU (>'73), Ziegler@Calgary(+) (>'75)
  - 80s: support industry for catalysis Mitsui, Shell, Akzo, Unilever

- 22 people (15 senior PhD's) + 3 EU fellows
  - New development, support, document, optimize

- Many collaborations non-profit & commercial
  - 160+ authors
  - New functionality, real-life pilot cases

- 1000s of users academia, government & industry



Bottom up Property Prediction

Properties are determined at the atomistic level => predict, understand & improve through modeling

Batteries: fast recharge, high capacity

Materials: light & durable
Paint/glass: optical properties, coating

Reduce friction

Solar cells: long lifetime & high efficiency

Bottom up Property Prediction

Atomistic modeling
- Decreases search space
- Builds understanding

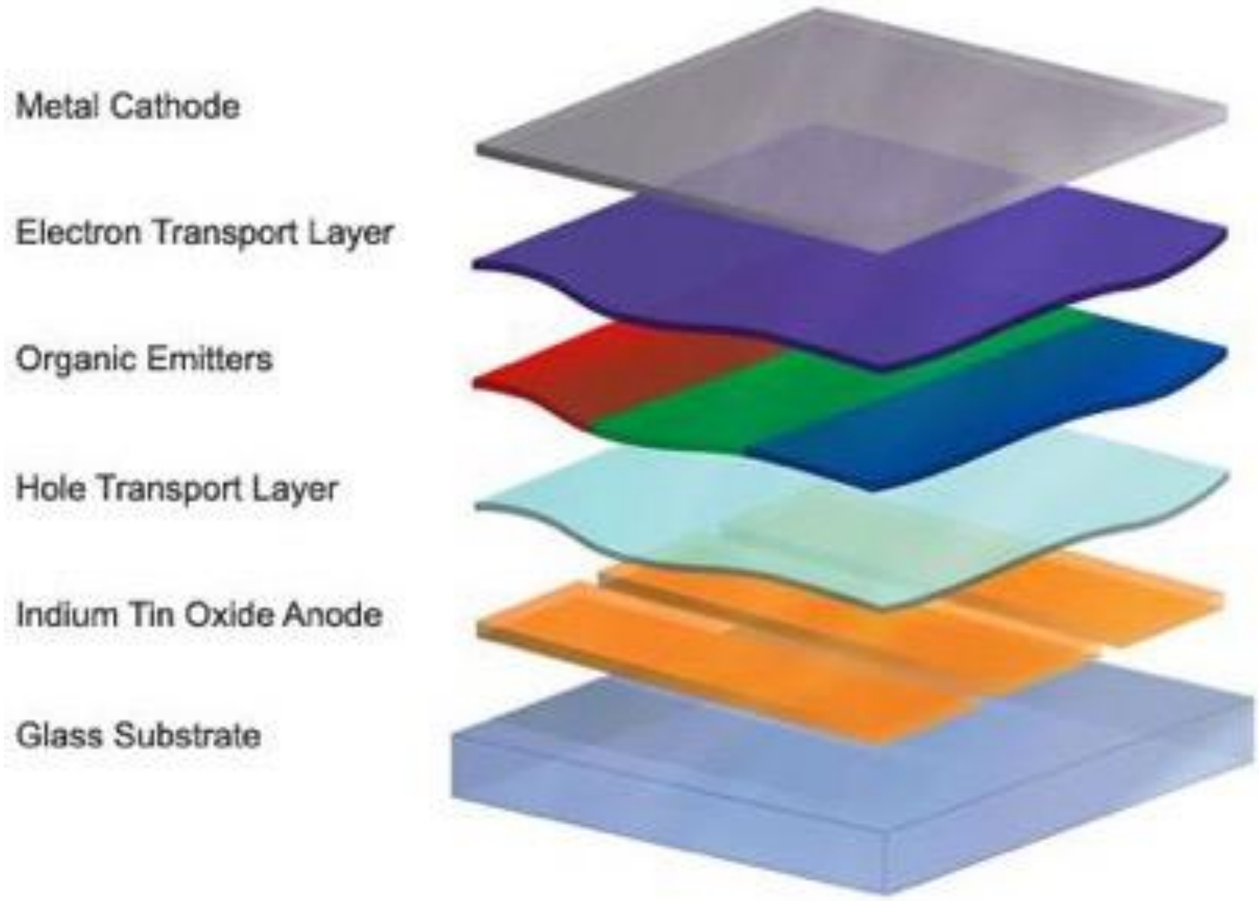
Batteries: fast recharge, high capacity

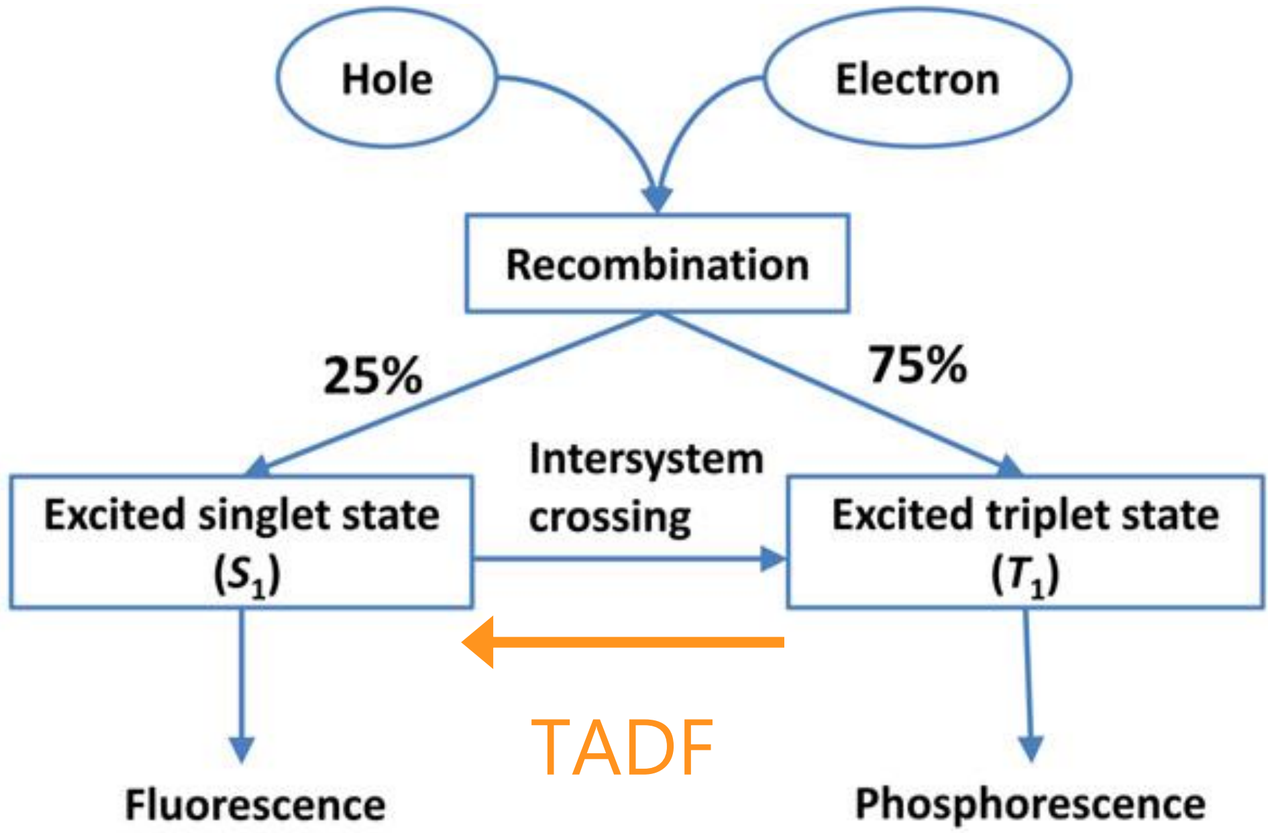
(m)CPU: high capacity, I-V profiles

Glass, coating: optical properties, conductivity

OLEDs, QLEDs: color, lifetime & efficiency

OLEDs: Optimize many materials & properties

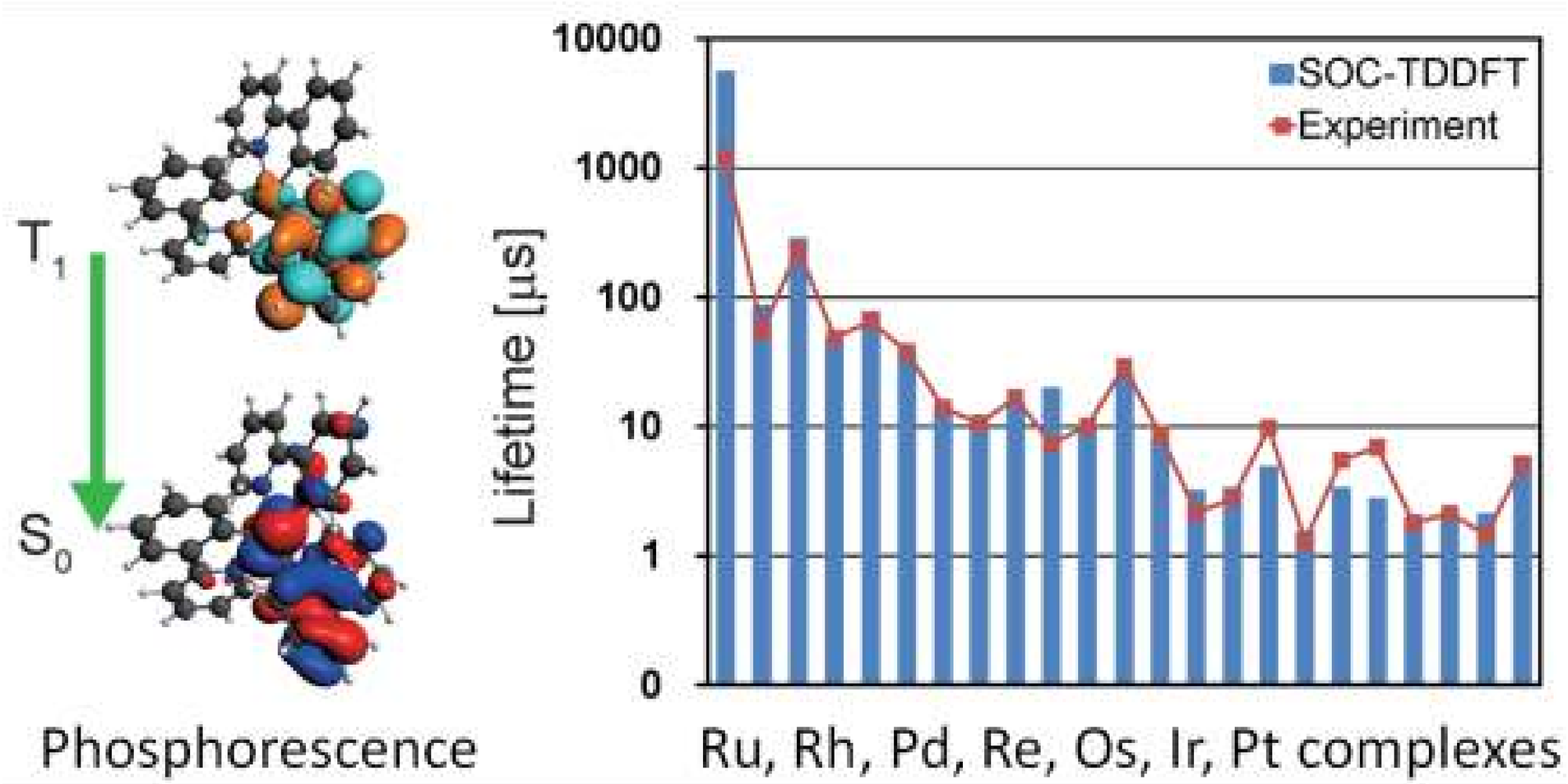




- Maximize luminescence
- Optimize color
- Minimize destructive processes
- Optimize charge & exciton transport

Optimize OLED emitter lifetimes

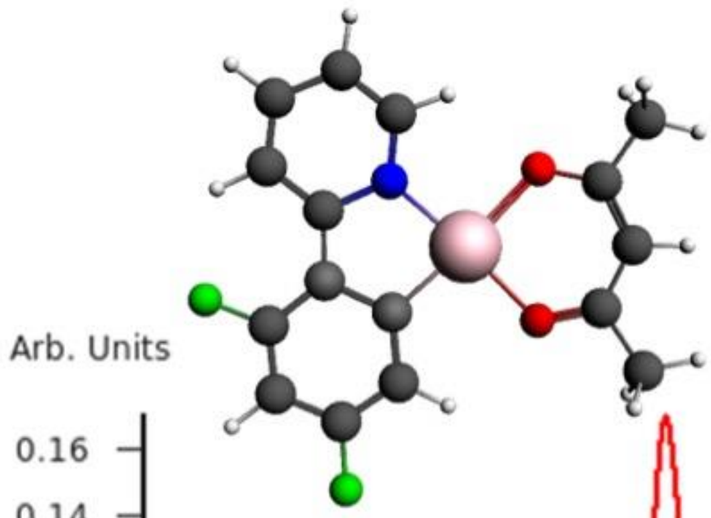
ADF 2005: Spin-orbit TDDFT => phosphorescence lifetimes

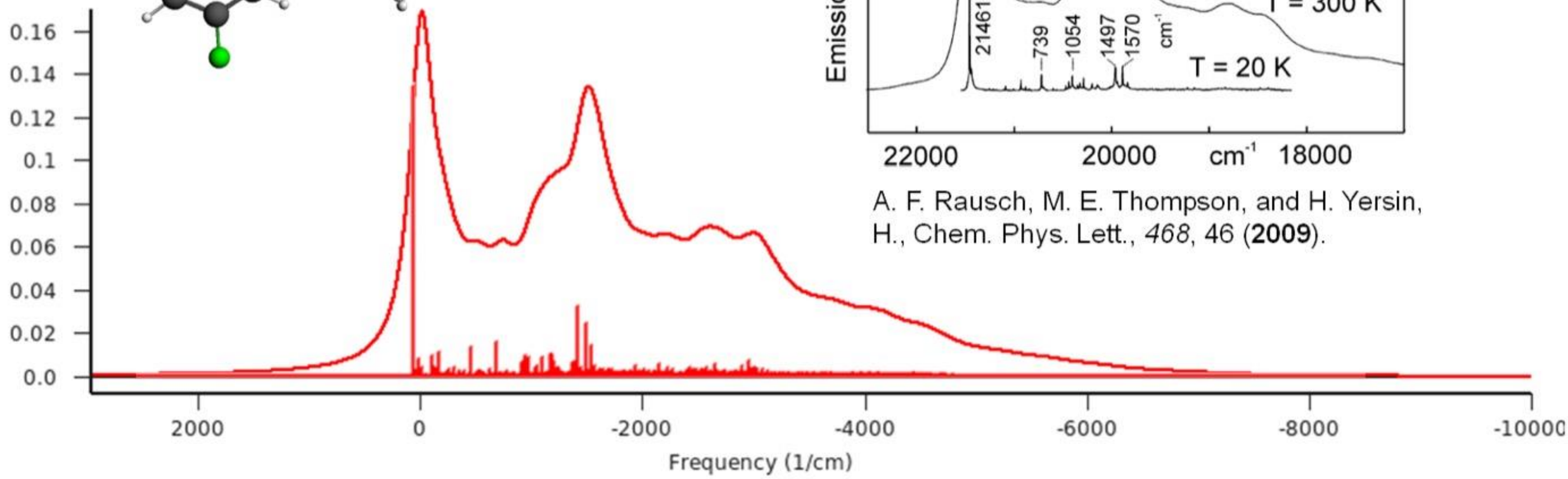


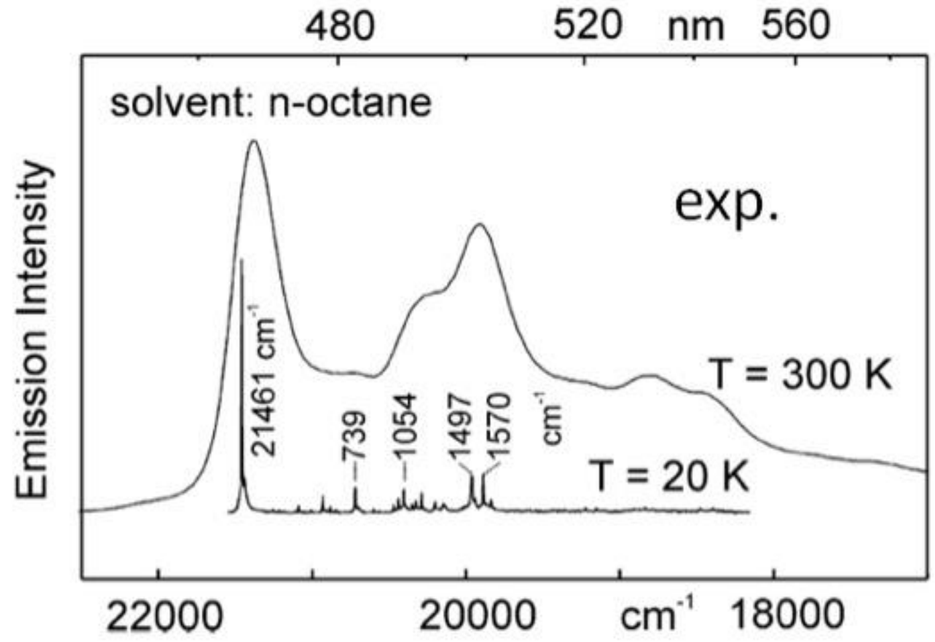
PCCP 16, 14523 (2014)

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

Optimize OLED emitter color / emission width







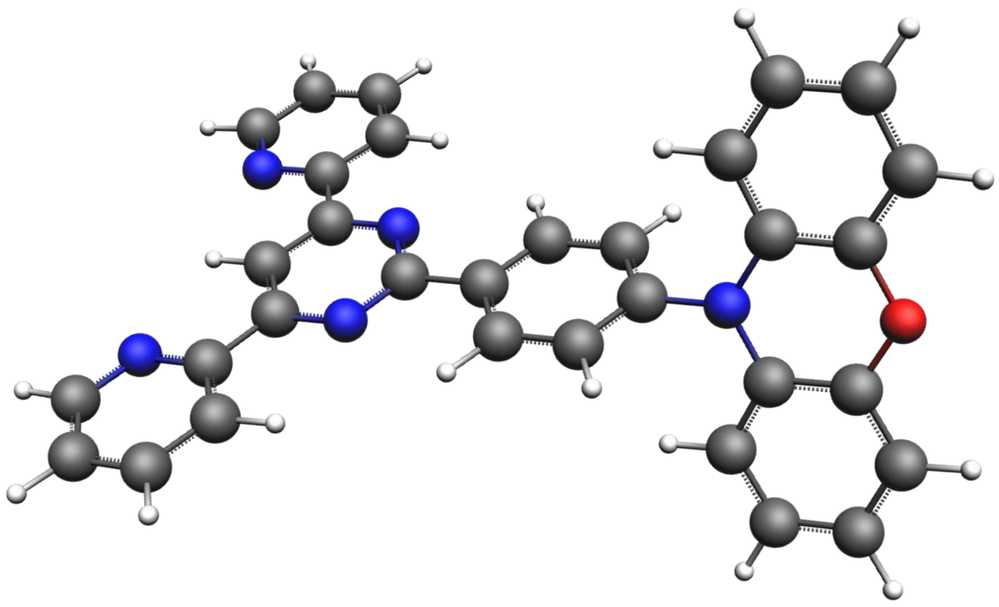
A. F. Rausch, M. E. Thompson, and H. Yersin, H., Chem. Phys. Lett., *468*, 46 (**2009**).

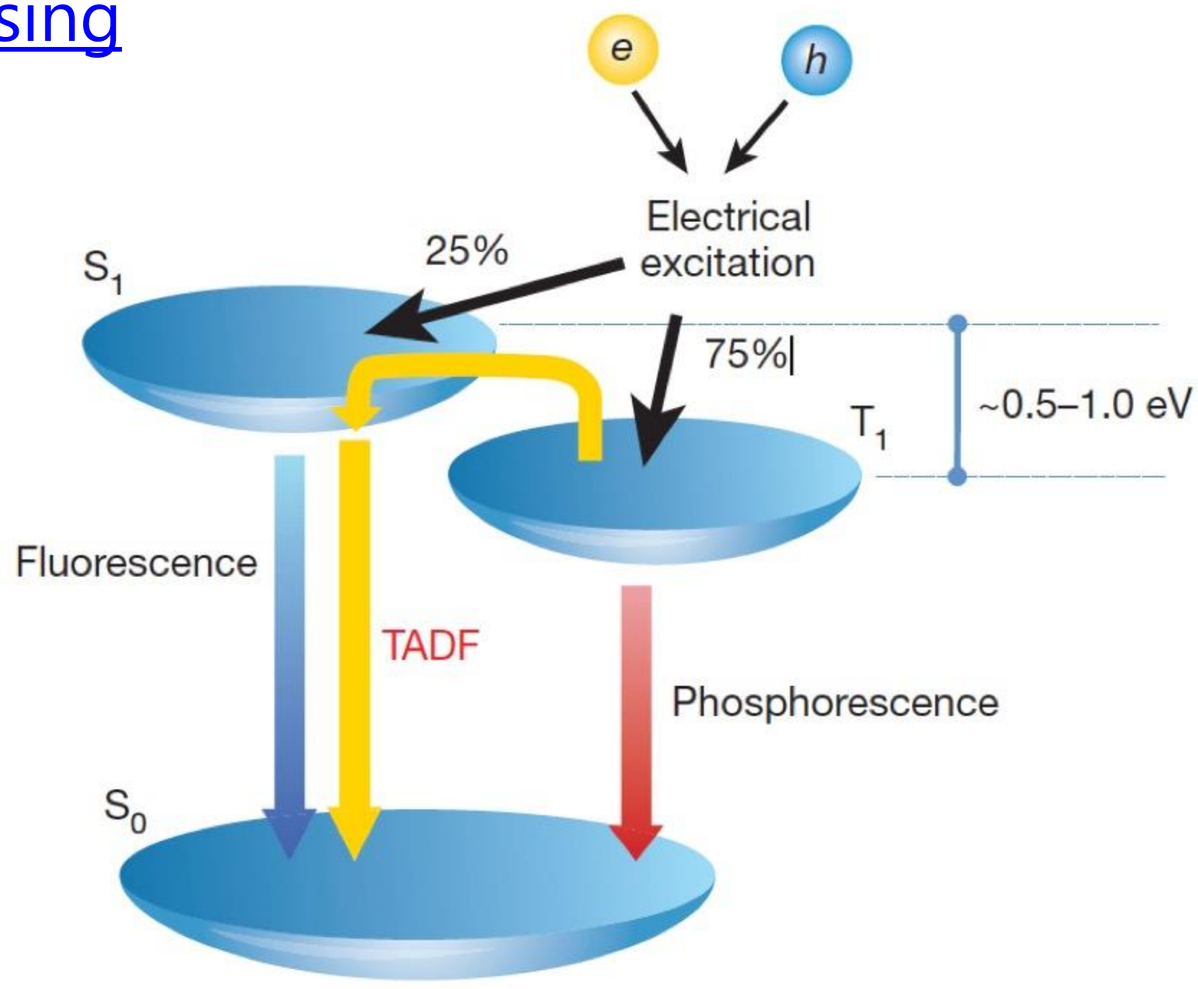
- Excellent agreement vibrational progression FCF T_1-S_0
- 0-0 well reproduced by Delta SCF calculation (22,000 cm^{-1})

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

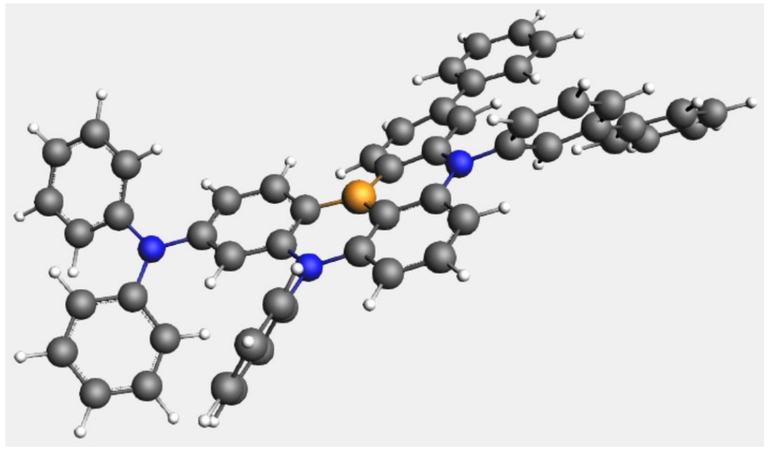
Forward vs. inverse property prediction

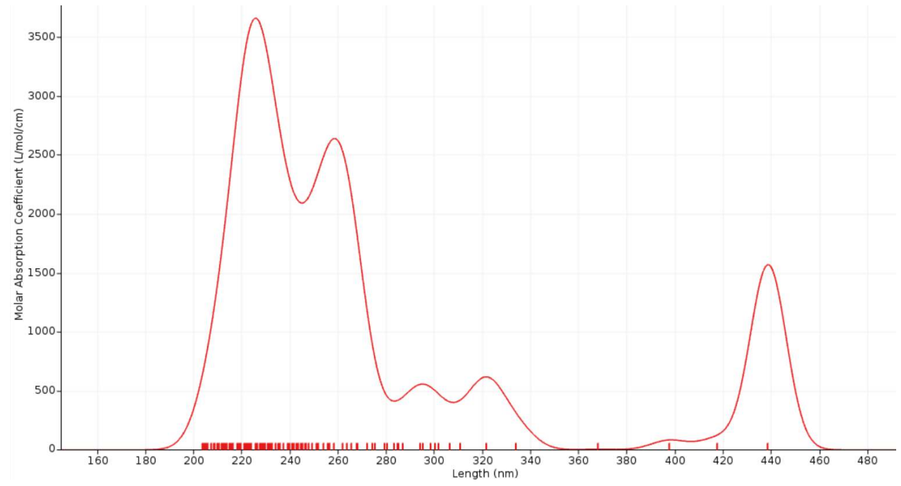
Forward prediction

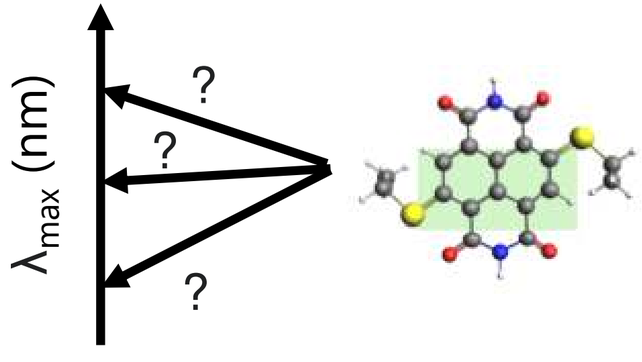
- Structure => property
- High-throughput (costly)
- ‘Stupid’, inside-box design

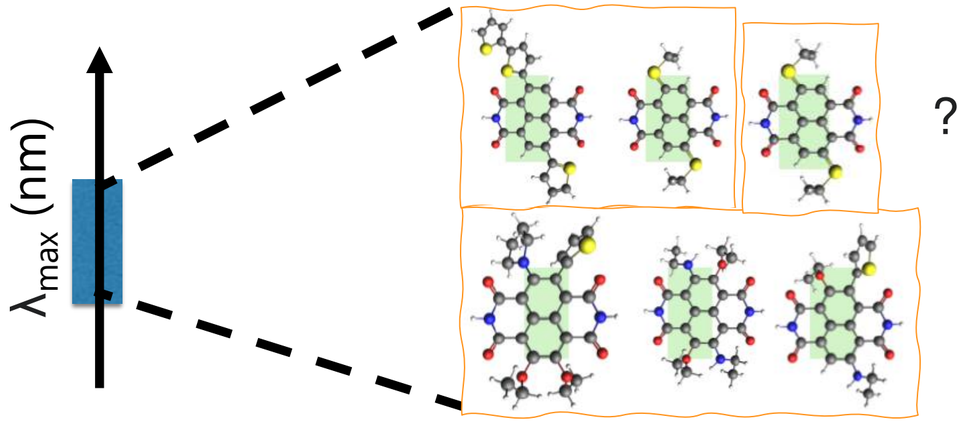
Inverse prediction

- Target desired property
- Encode properties to (sub)structures
- Include constraints & boundaries



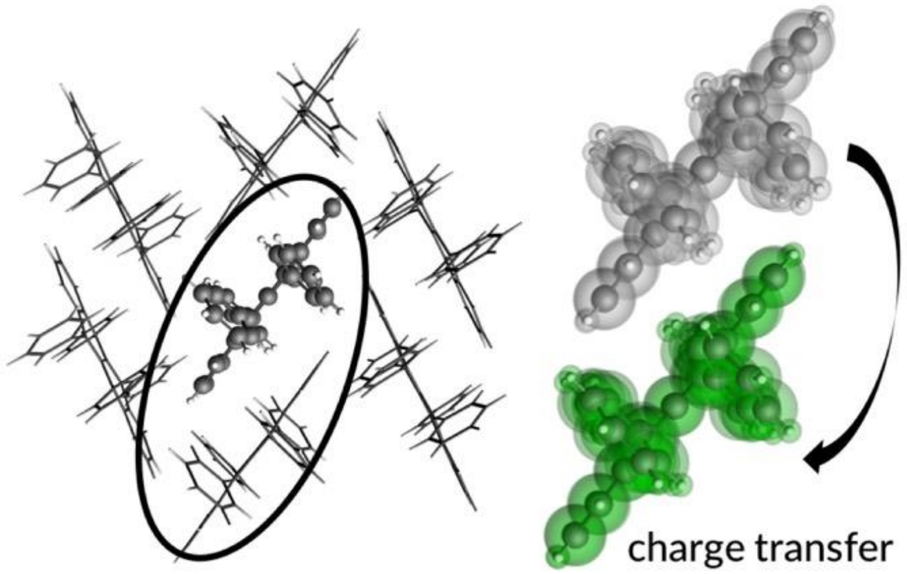


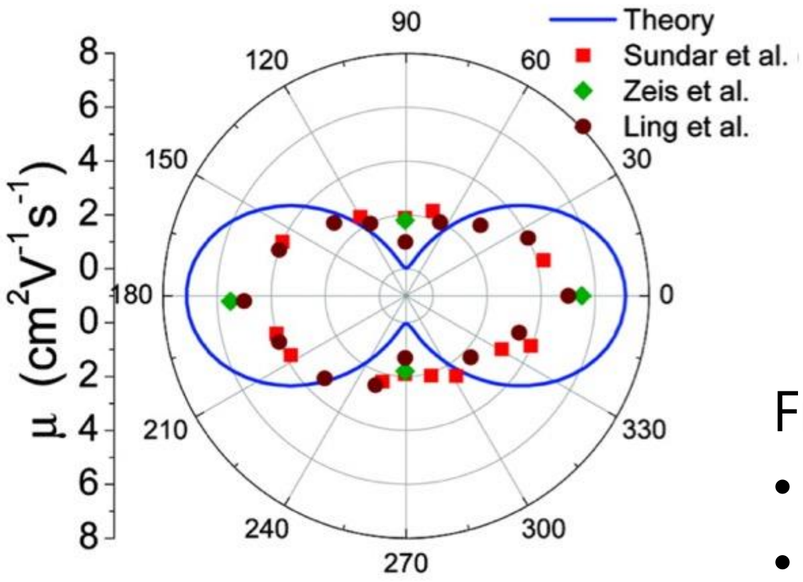




Optimize charge mobility (OLED, OFET)

- 2003: easy to get transfer integrals from ADF (fragment-based)
- 2007: organic semiconductors (**BASF**): hole and electron mobility





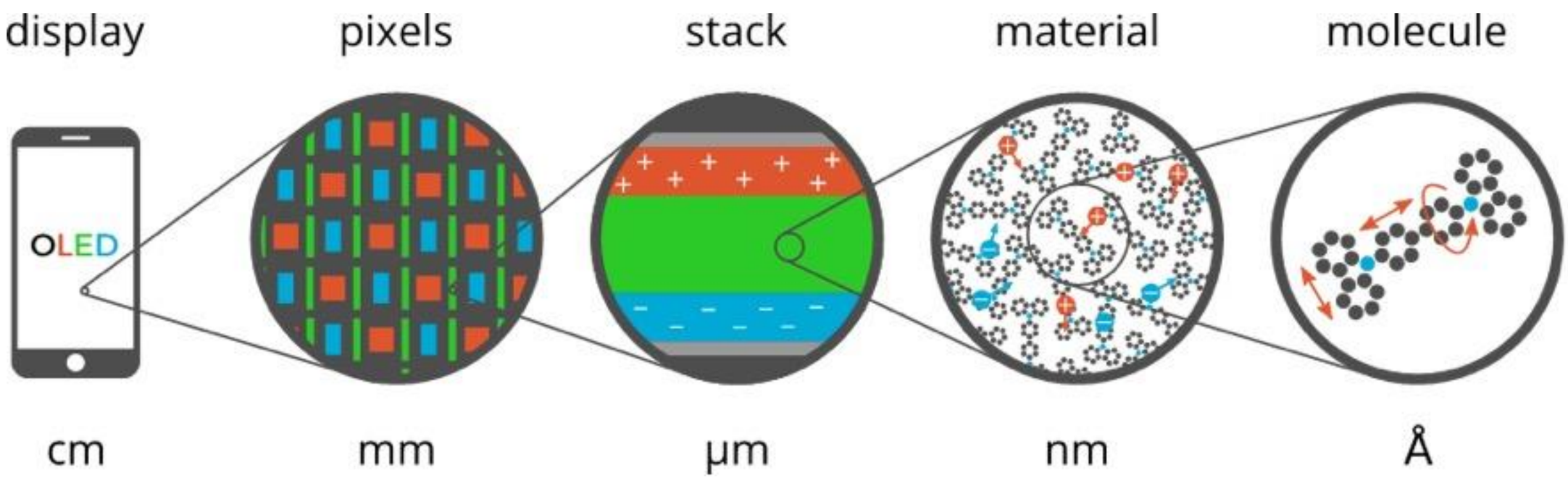
From adiabatic states

- Environment polarization
- Charge generation
- Charge recombination
- Exciton transfer

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

Extending to device modeling

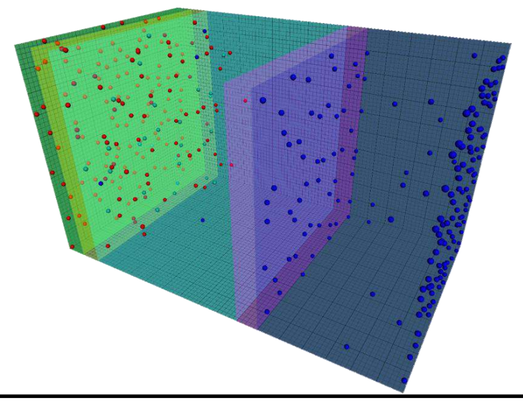
- New collaboration SIMBEYOND



- Integrate Atomistic with Device Modeling => Single platform

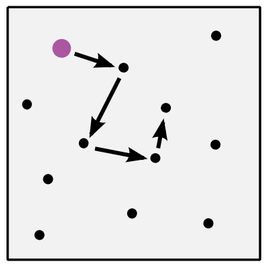
bumblebee™

  - kinetic Monte Carlo, full 3D device model
  - electronic and excitonic processes

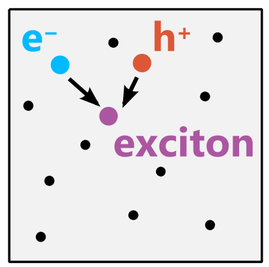


Device-level physics

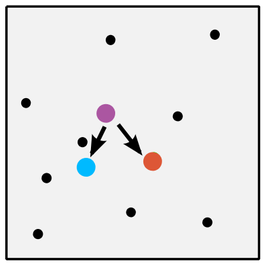
- Electronic processes
  - Charge injection, hopping and collection
  - Coulomb interactions, external fields and image potential
- Excitonic processes



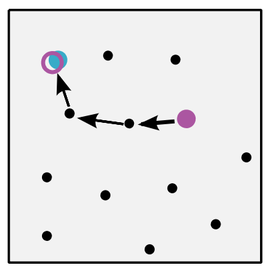
Exciton diffusion:
– Förster
– Dexter



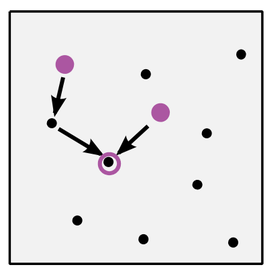
Exciton generation



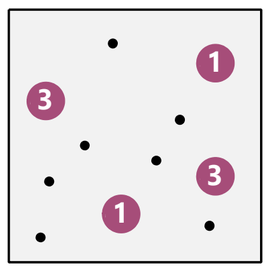
Exciton dissociation



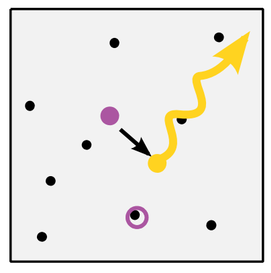
Exciton-polaron quenching



Exciton-exciton annihilation



(Reverse) Inter-system crossing

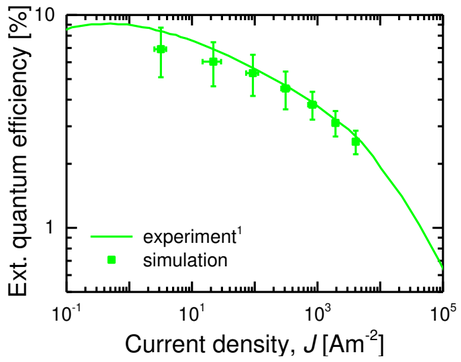


(Non-)radiative decay

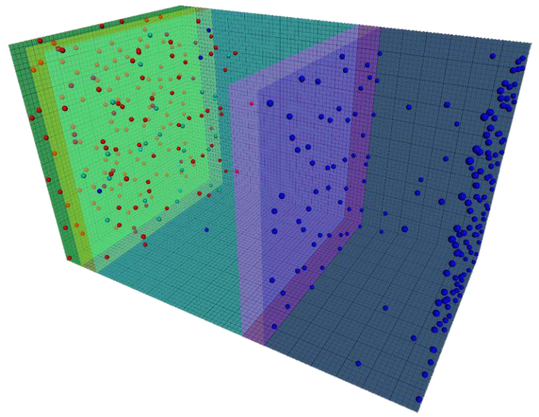
- Degradation processes

Device-level predictions & insights

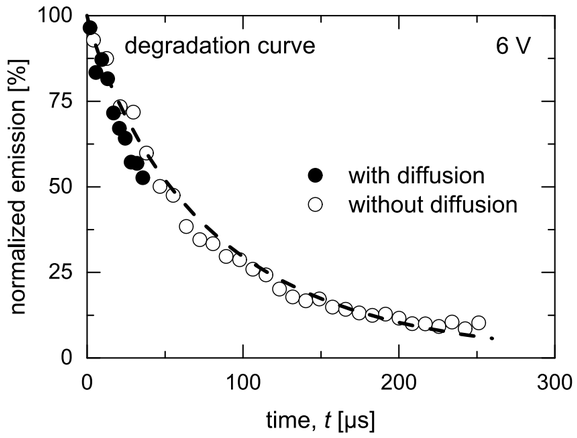
Efficiency roll-off



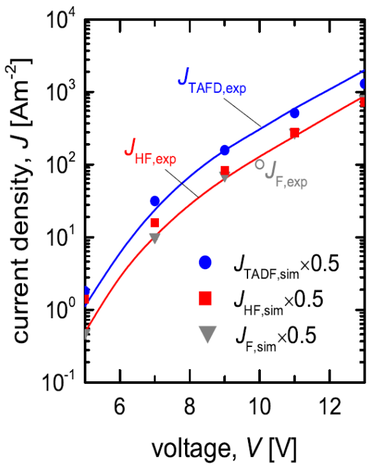
3D visualization



Device lifetime

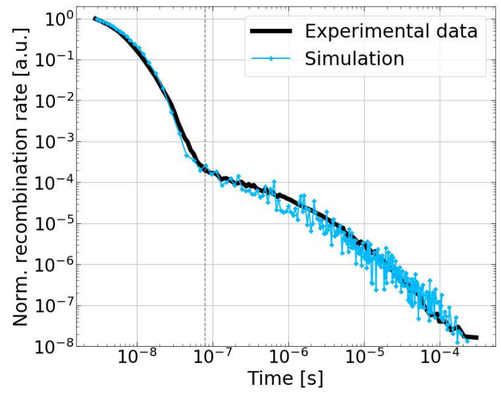


$J(V)$ characteristics

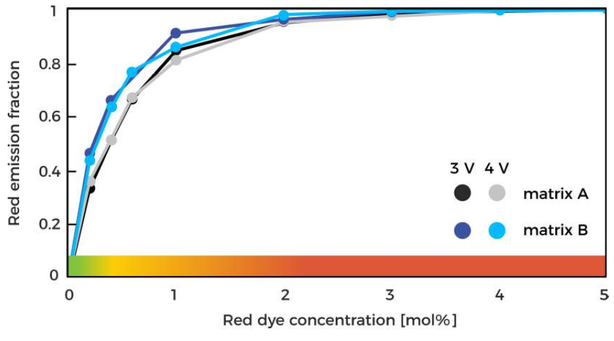


bumblebee™

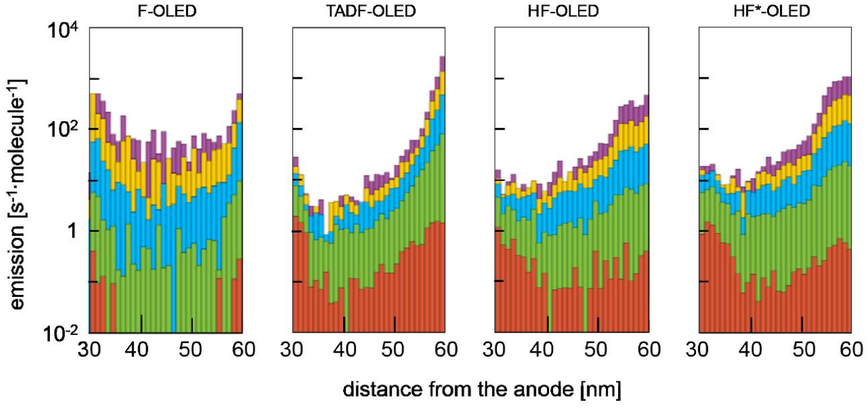
Transient behavior



Color point shifts



Profiles

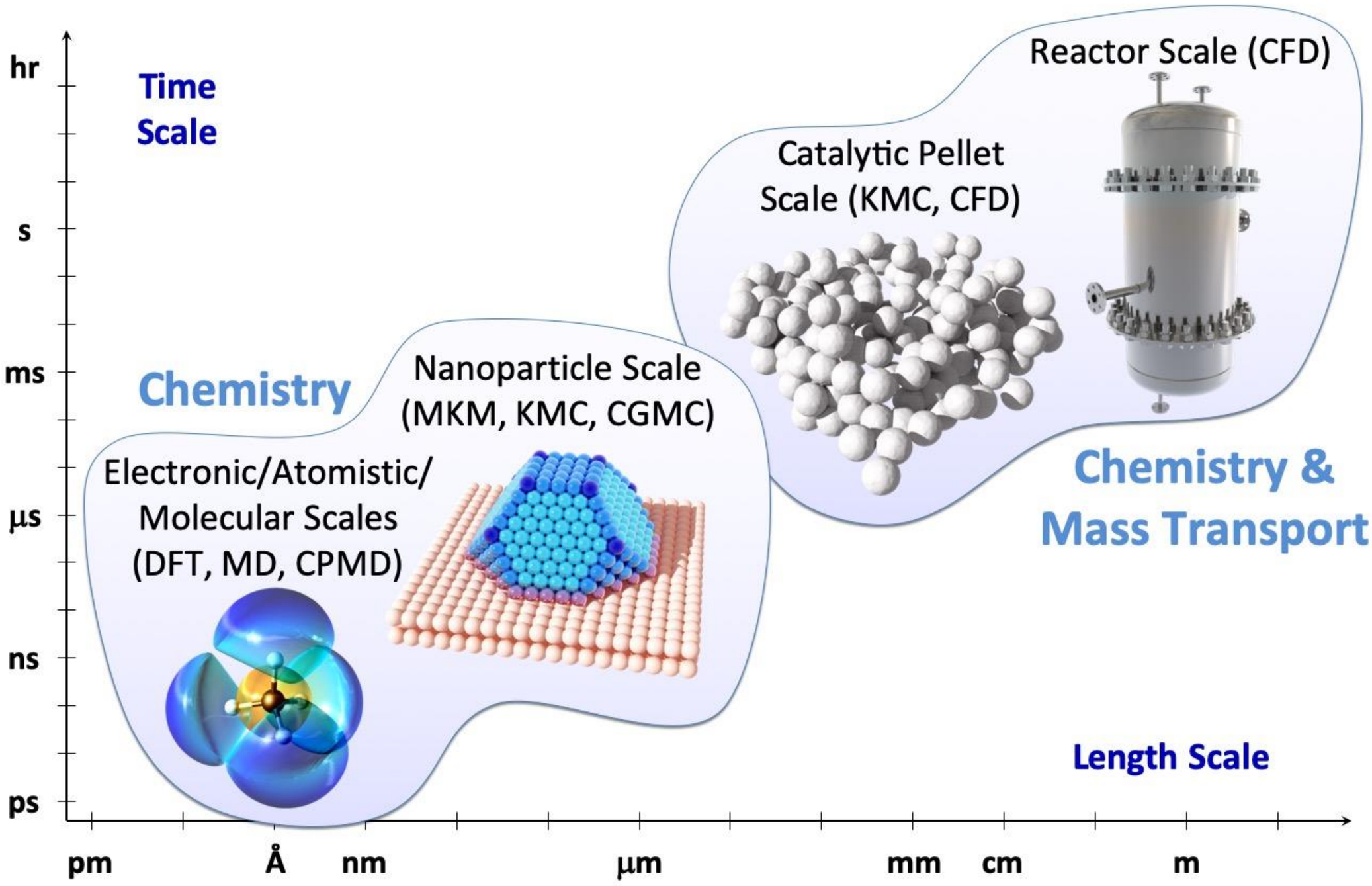


Nature Mater. **12**, 652 (2013)
Appl. Phys. Lett. **105**, 143303 (2014)
Adv. Funct. Mater. **25**, 2024–2037 (2015)
Appl. Phys. Lett. **114**, 073301 (2019)

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

SCM

ReaxPro: Reactive Materials & Process Design as a Multi-scale / Multi-equation Problem



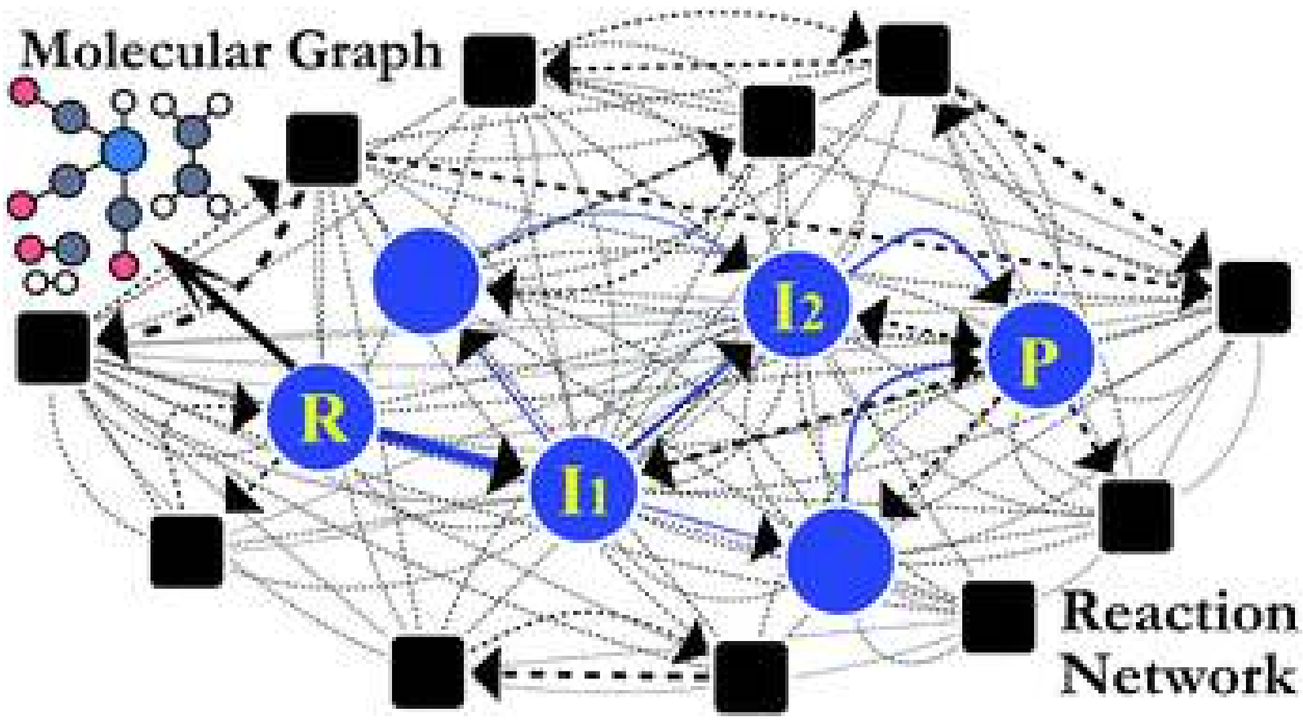
Industrial partners: BASF, JM, DowDuPont, Shell

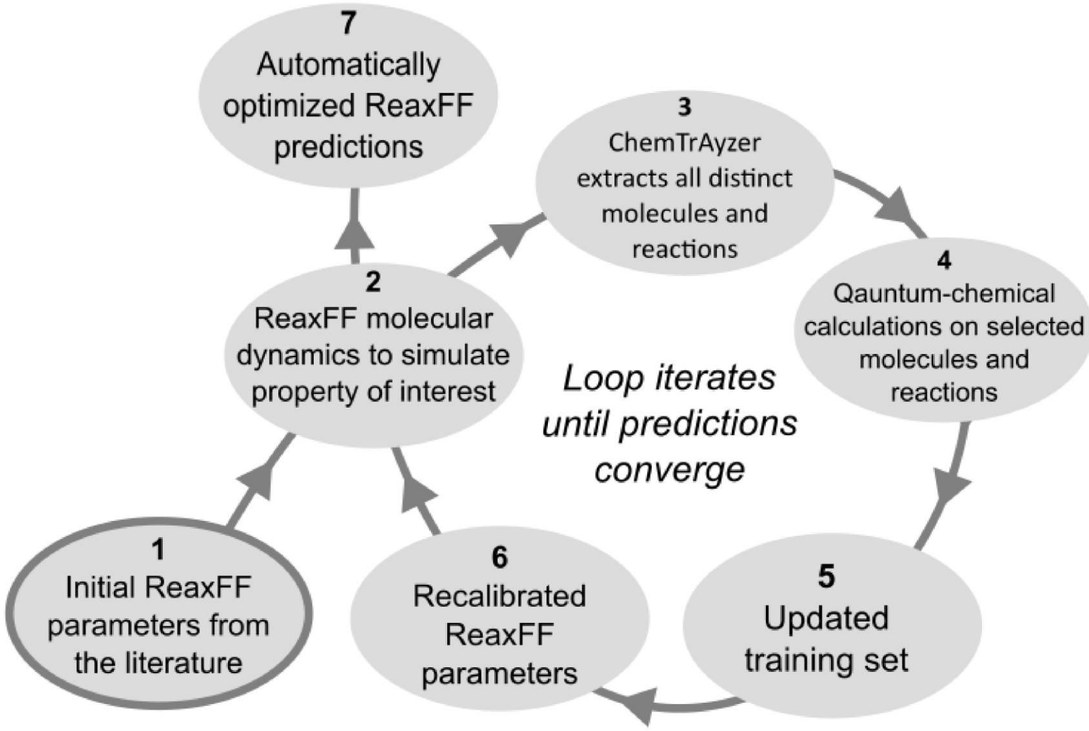
MD: EON, kMC: Zacros, CFD: Catalytic FOAM

AutoCheMo: Automatic generation of Chemical Models

4 PhD projects, in collaboration with Universities of Gent and Aachen:

- Complex reaction networks
- Application-driven automated ReaxFF force field parameterization
- Efficient (Bayesian) methods to estimate ReaxFF parameters
- Large amplitude motions

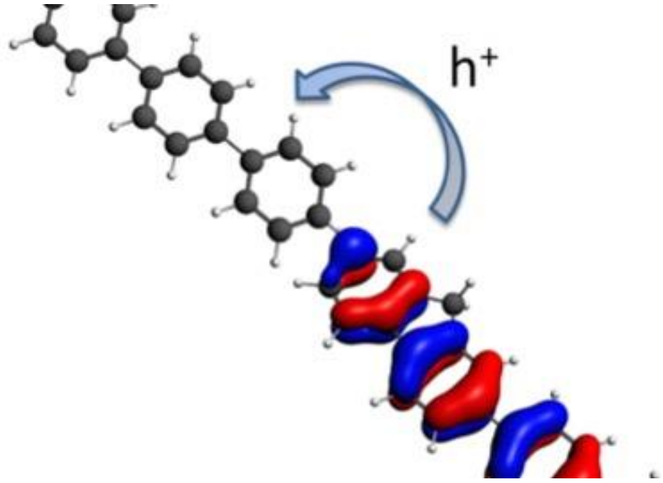




Also working with KAIST on ACE-Reaction (now also working on machine learning)
Y. Kim, J. W. Kim, Z. Kim and W. Y. Kim, Chem. Sci. 2018, 9, 825; JPCA 2019, 123, 4796.

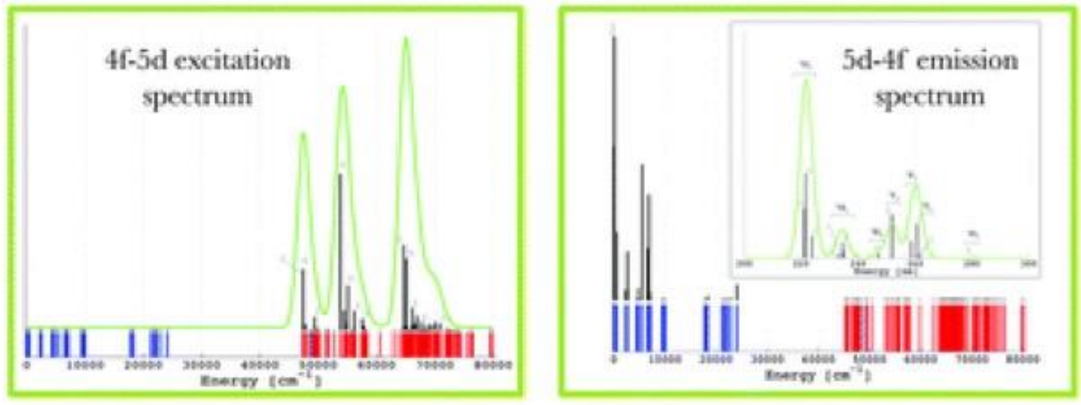
Modeling display materials

- Charge mobility
  - ADF: transfer integrals, couplings through FDE
  - ADF: NEGF (single-molecule junction)
  - ADF: charge transfer descriptors
  - BAND: effective mass (band transport)



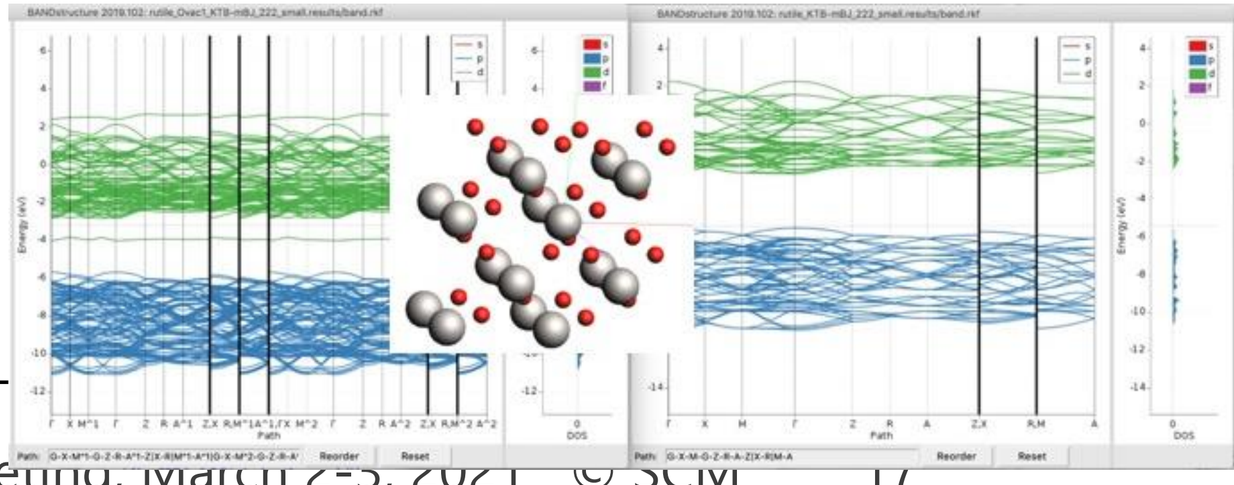
- Luminescence, including phosphorescence
  - ADF: spin-orbit coupling TDDFT
    (k_phos, k_RISC for TADF, vibronic fine structure)
  - LFDFT: luminescence of Ln-doped ceramics
  - BAND: core-hole states in bulk / surfaces
  - ADF: quantum dots – fast TDDFT methods

Two-open-shell **LFDFT** calculation of $LiYF_4:Pr^{3+}$



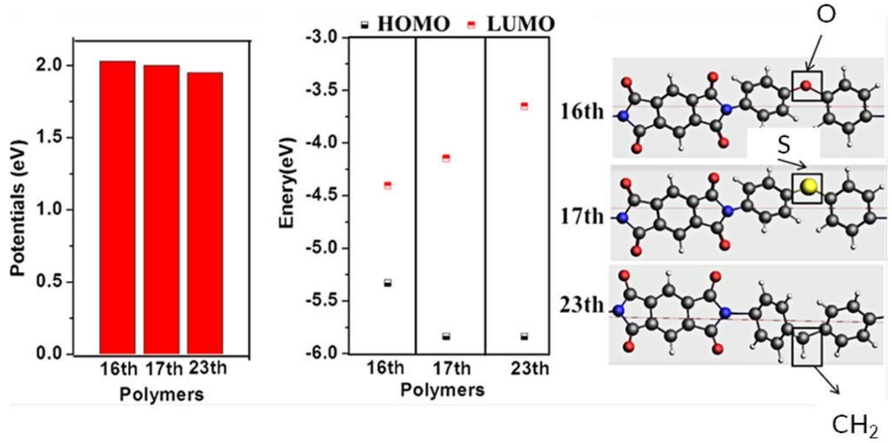
- (Non-radiative decay, exciton mobility, exciton-phonon coupling, ...

- BAND: band gaps, work functions
  - Proper 2D: solvation, E field, polarization

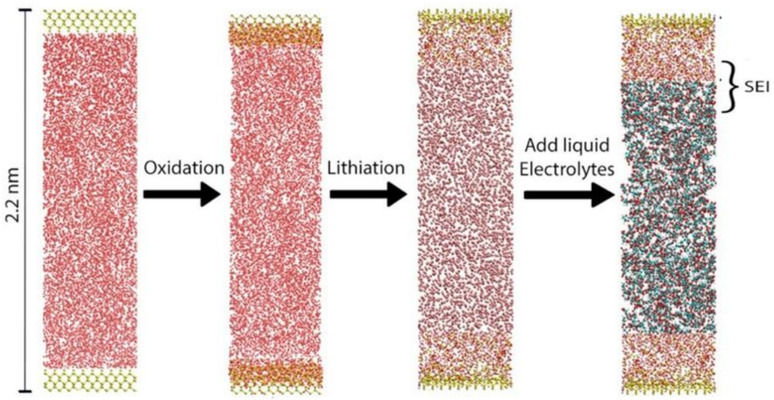


Modeling battery materials

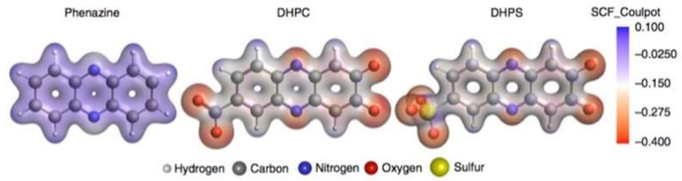
- Charge mobility
  - BAND: include solvation
  - eReaxFF, APPLE&P, polarizable force fields with MD
  - NEGF: mobility across interface



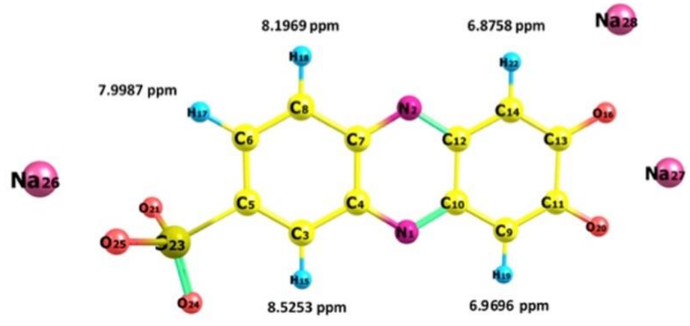
- Electrolyte solubility & reactivity
  - COSMO-RS for ionic liquids
  - (e)ReaxFF: electrolyte degradation
  - ReaxFF, DFTB, BAND, polymer properties



- (Dis)charge processes
  - GCMC with ReaxFF, or DFT(B)

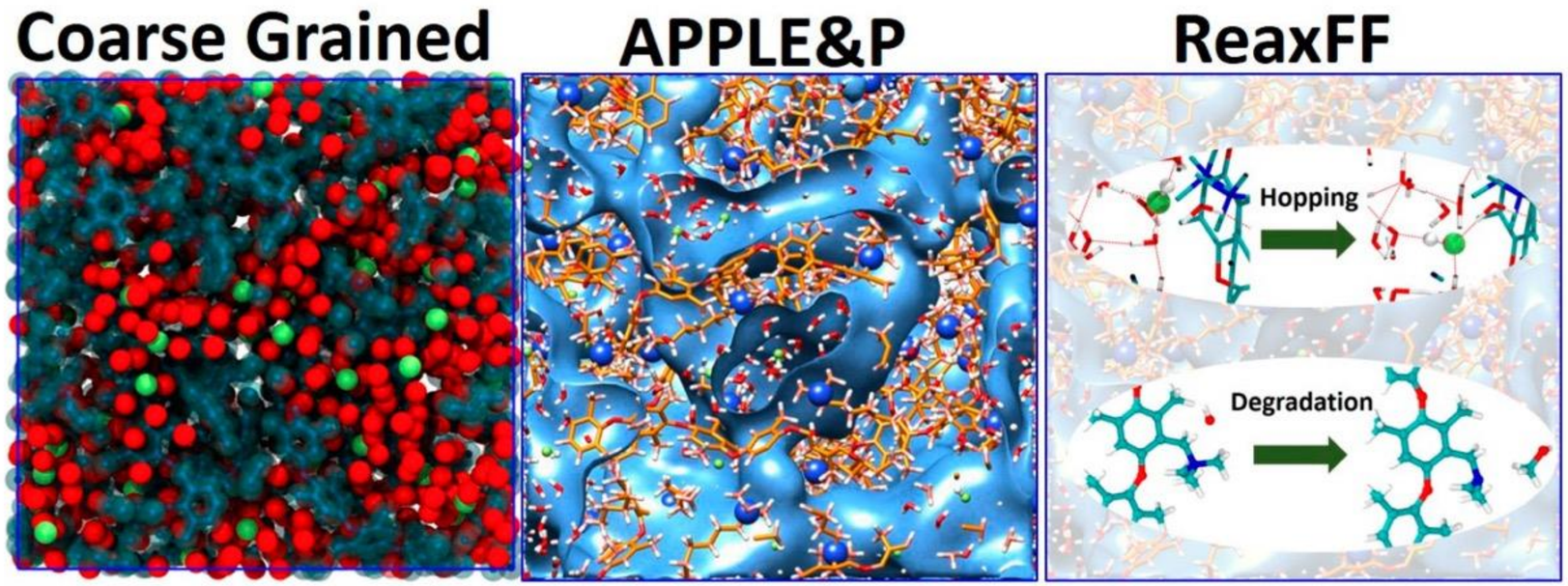


- Understand battery ‘operando’
  - ADF - Spectrocscopy: NMR, NEXAFS



Extending to larger scales

- New collaboration

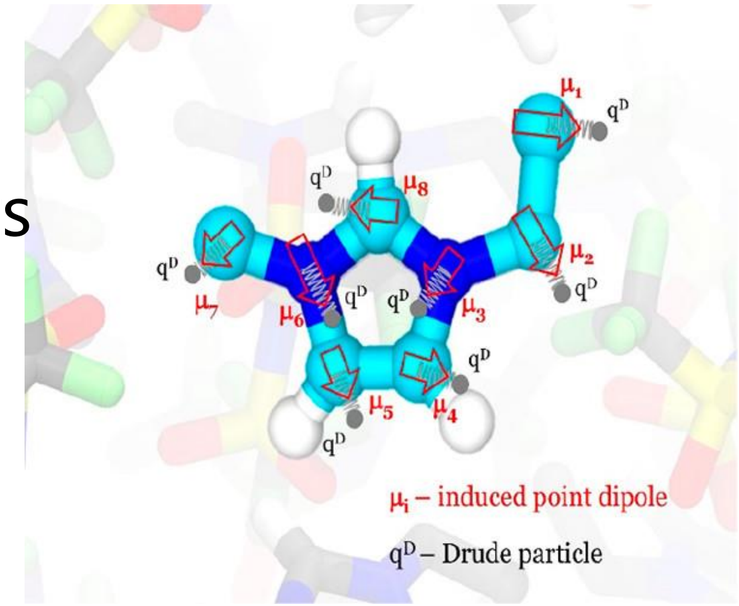


- Atomistic to meso-scale Coarse Grained => Polarizable -> Reactive FF

- Applications to **batteries** and **fuel cells**
  - Fuel cell membranes: Polymers 2018, 10, 1289; doi:10.3390/polym10111289

Polarizable Force Fields (with WMI)

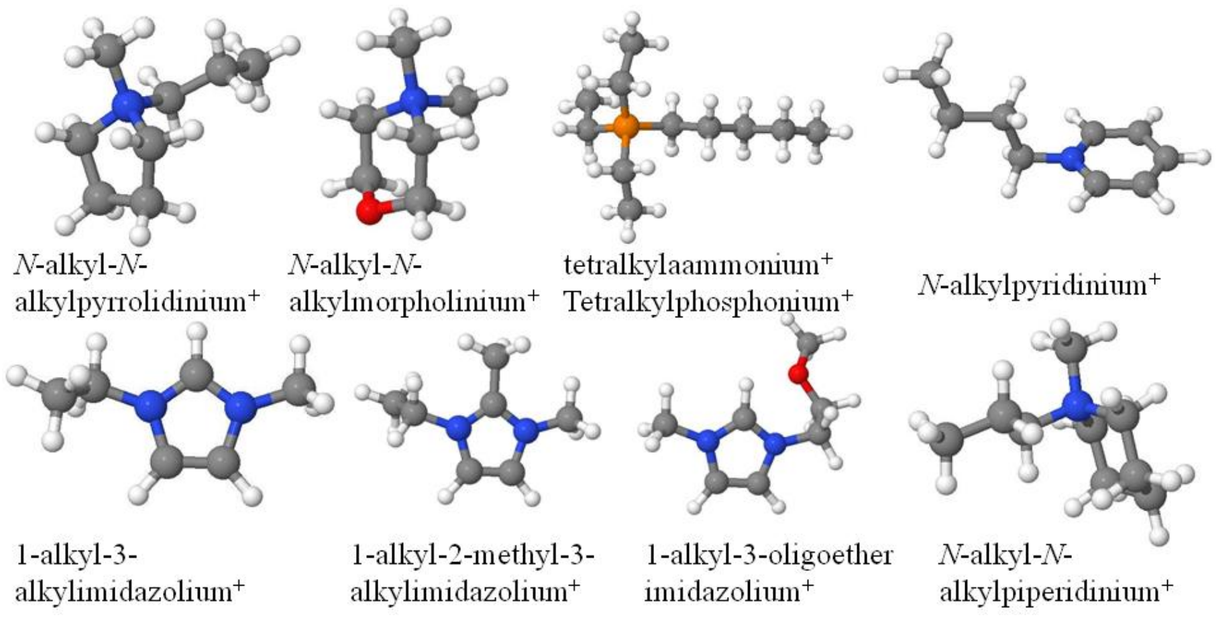
- Many-body interactions
- Transferable repulsion-dispersion + bond increments
- Thermodynamic & transport properties

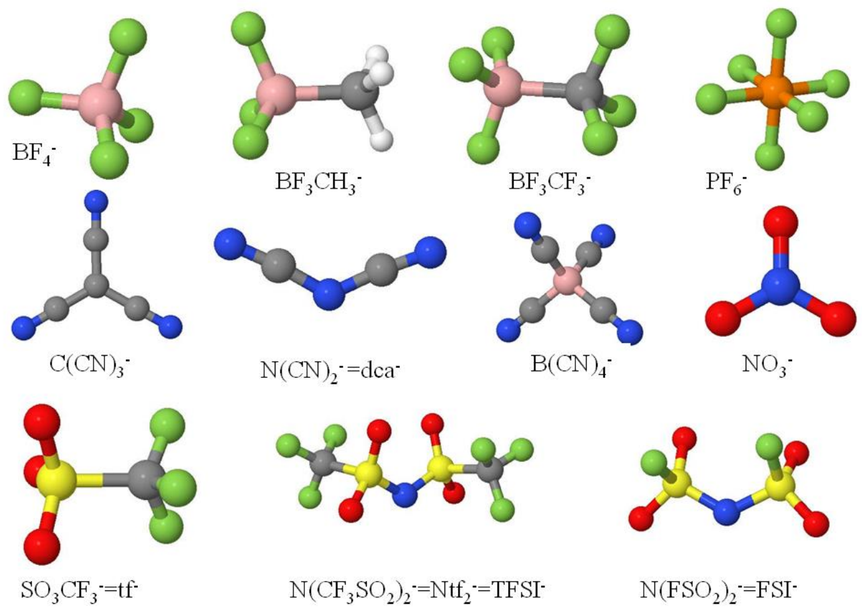


Chem. Rev. 2019, **119**, 7940

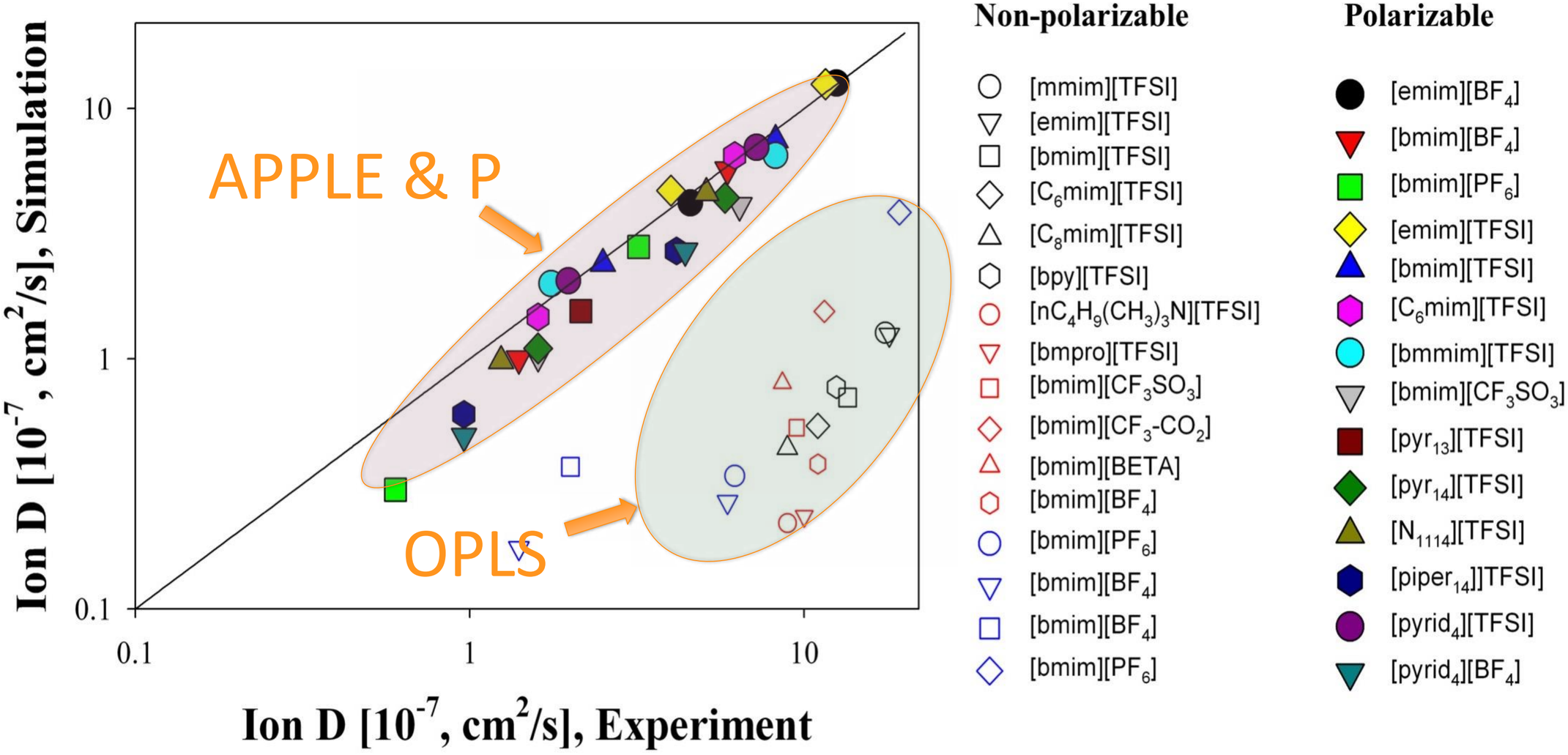
$$U^{NB}(r) = \sum_{i>j}\left(A_{\alpha\beta}\exp(-B_{\alpha\beta}r_{ij}) - C_{\alpha\beta}r_{ij}^{-6}\right) + \sum_{i>j}\left(\frac{q_i q_j}{4\pi\varepsilon_0 r_{ij}}\right) -0.5\sum_i \vec{\mu}_i \vec{E}_i^{\,0}$$

van der Waals — electrostatic





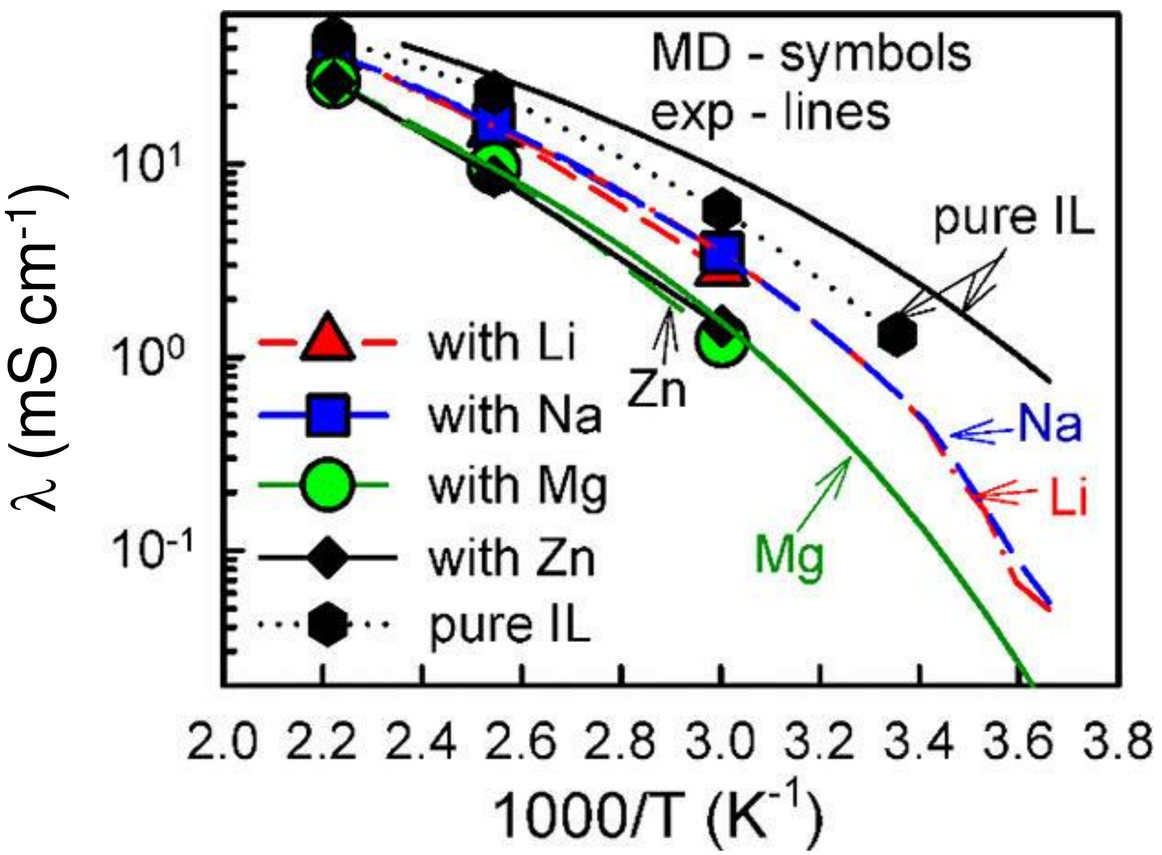
Self-diffusion coefficients of ILs

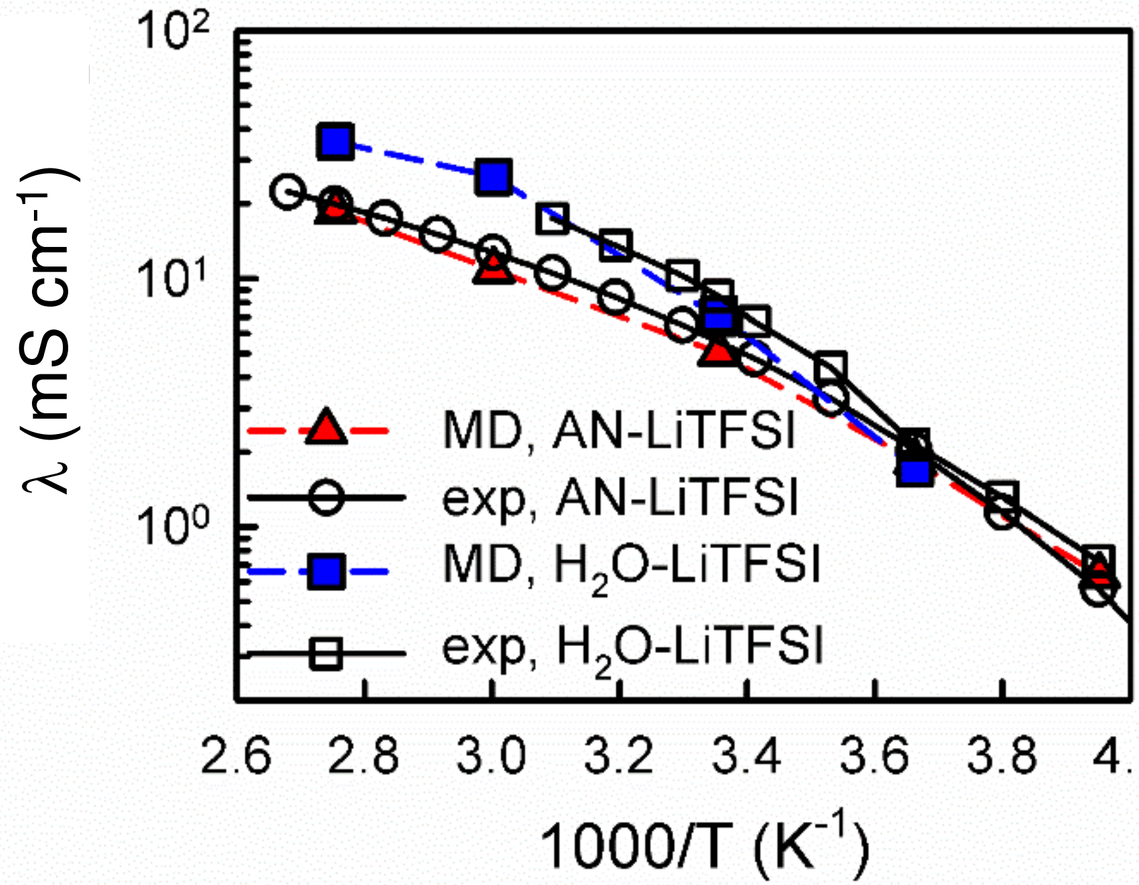


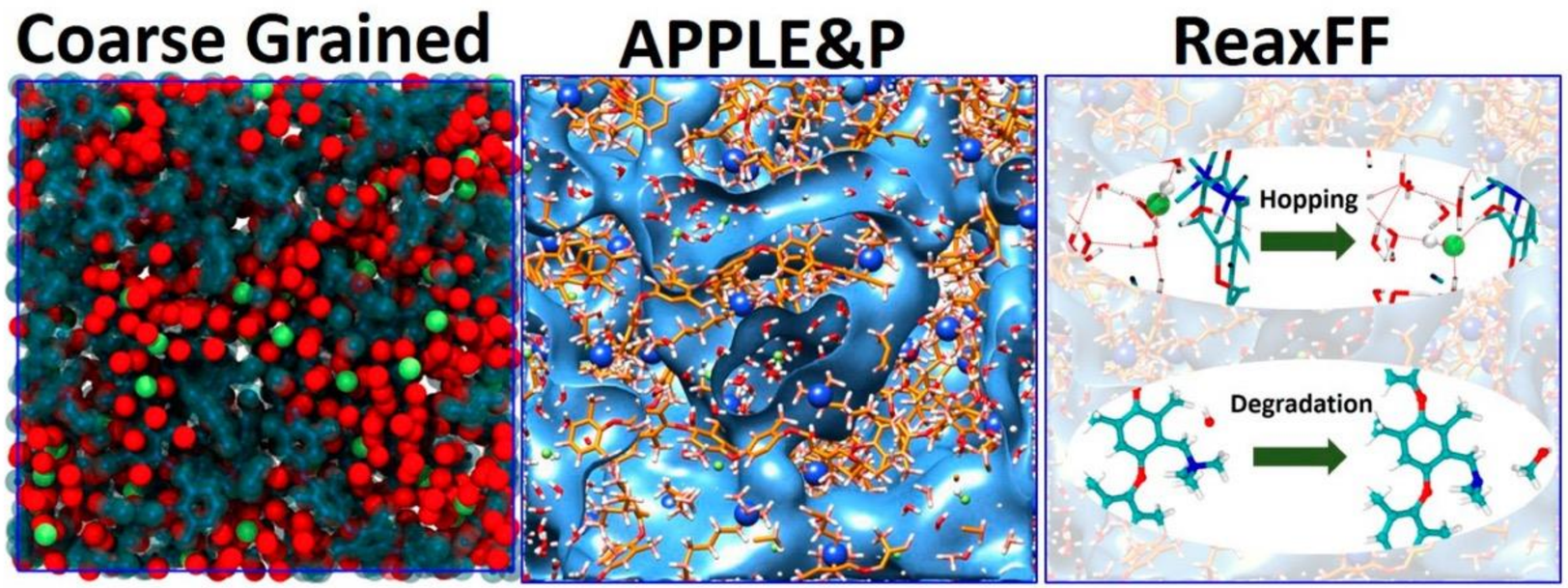
MD simulations using APPLE&P force field predict ion dynamics within 15-20% from experiment.

More transferable than “scaled” non-polarizable force fields with ion charges rescaled by 0.6-0.8.

Conductivity with APPLE&P => multiscale

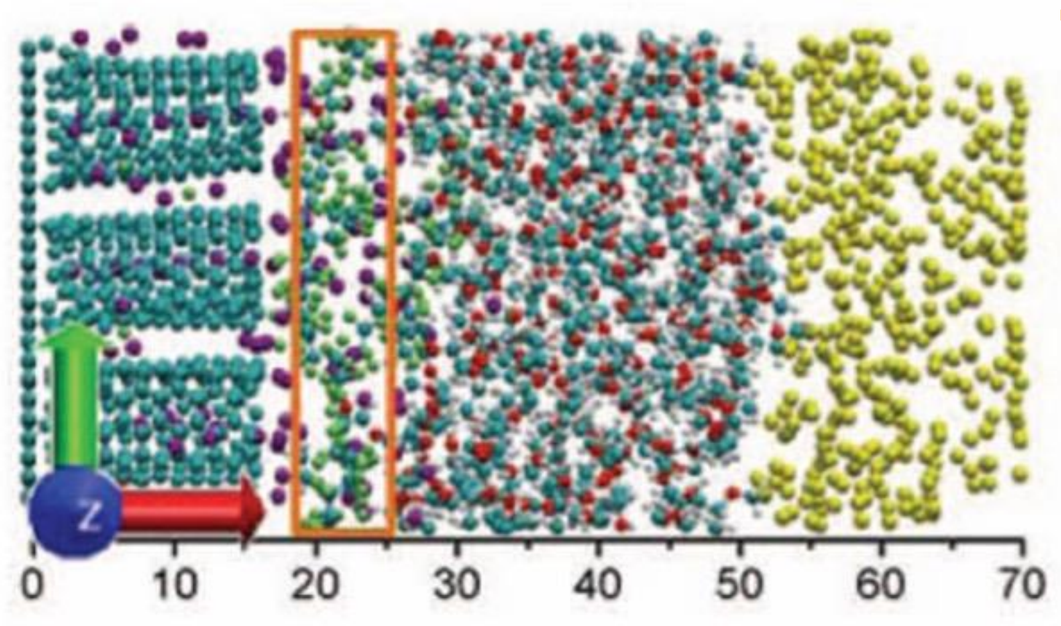




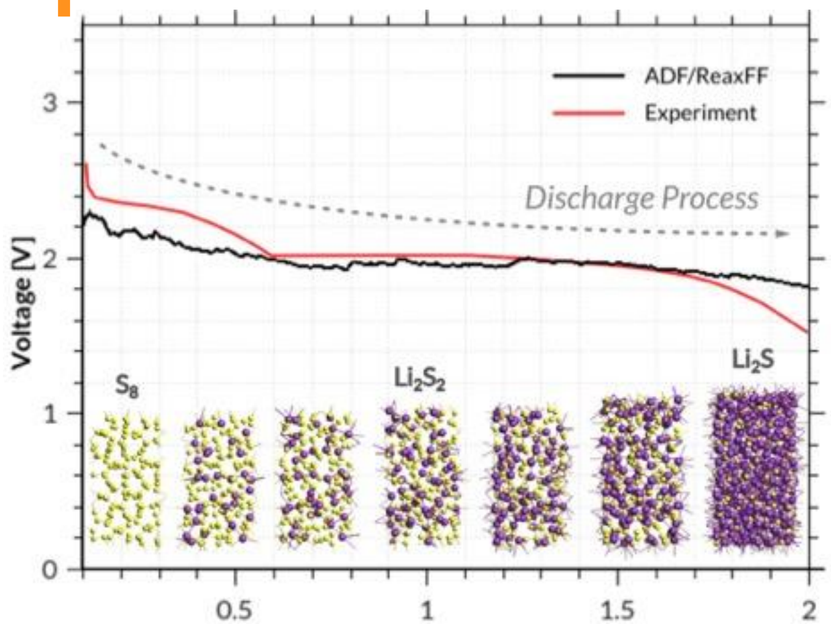


Wasatch Molecular INCORPORATED

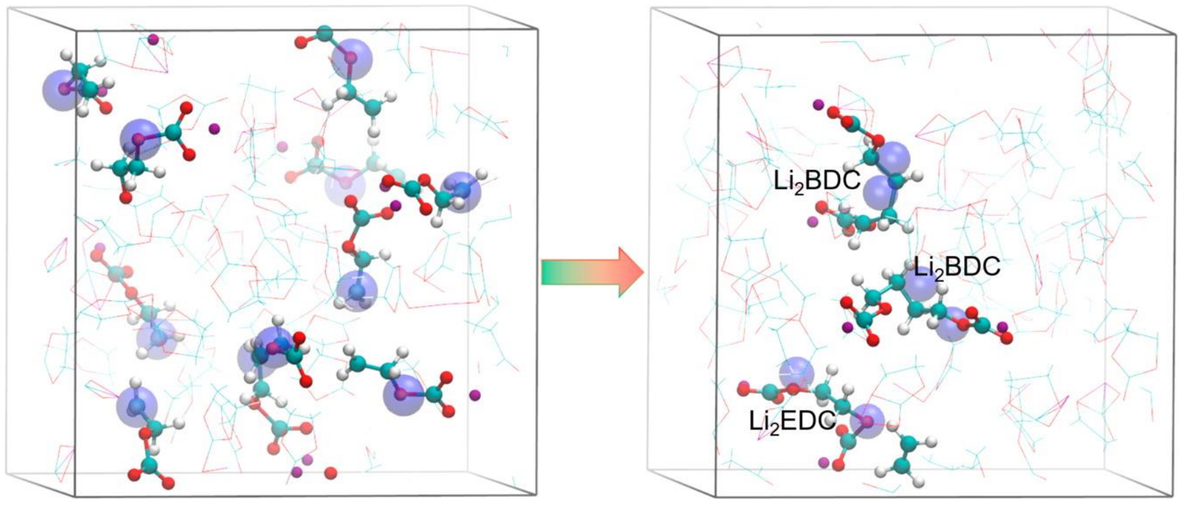
ReaxFF: battery applications



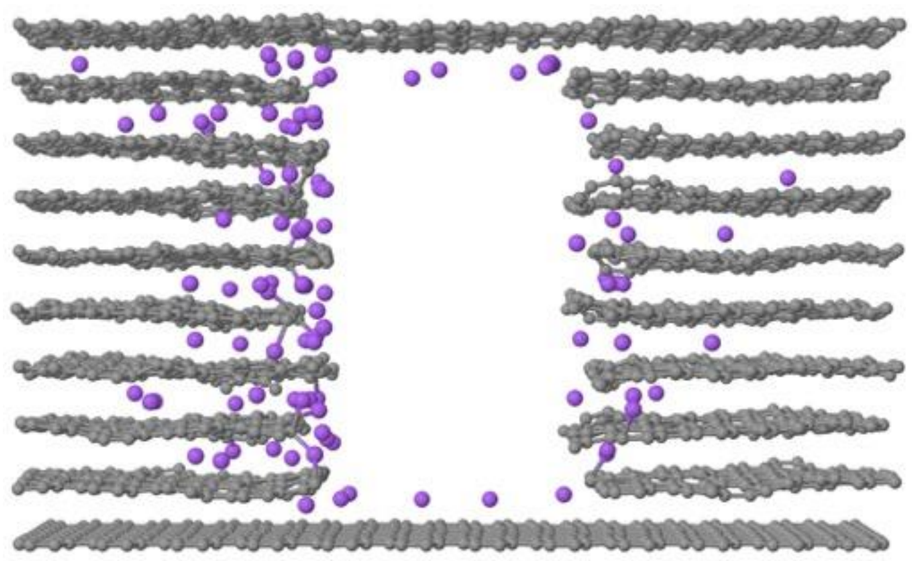
Teflon slows down Li in battery discharge
J. Electrochem. Soc. 161, E3009 (2014)



Sulphur cathode expands under discharge
PCCP, **17**, 3383 (2015); **Tutorial**



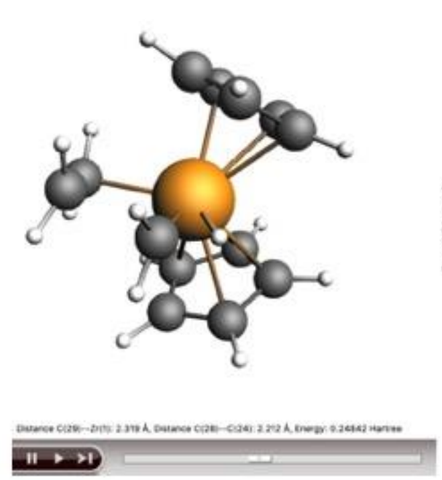
eReaxFF: electrolyte decomposition at the SEI
J. Phys. Chem. 120, 27128 (2016)

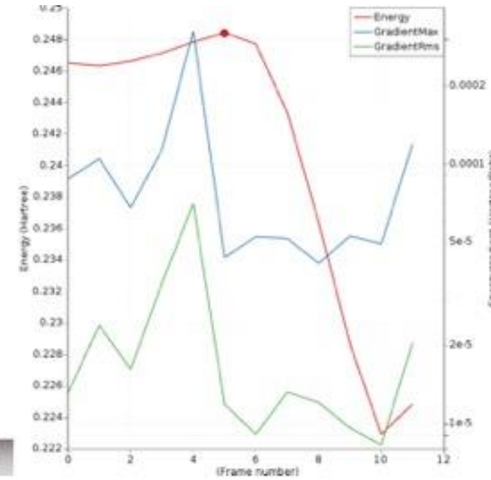


Sodium intercalates in graphitic cathodes
(new FF with MCFF) PCCP 18, 31431 (2016)

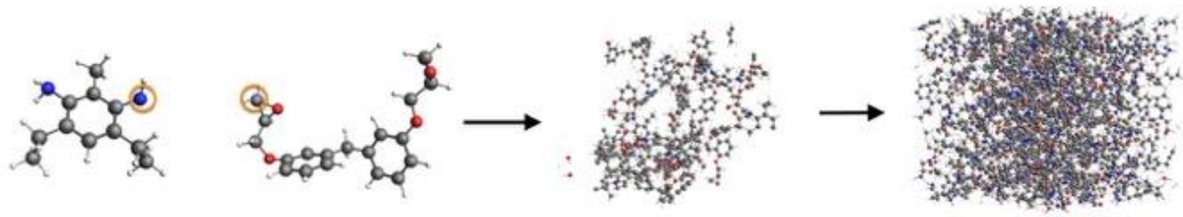
Modeling polymers

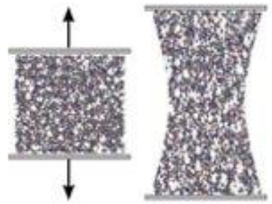
- Formation
  - Whole of AMS: catalysis
    - Reaction rates, spectroscopy, catalyst design
  - ReaxFF (bond boost): cross-linking
  - Solvent effects: COSMO(-RS)

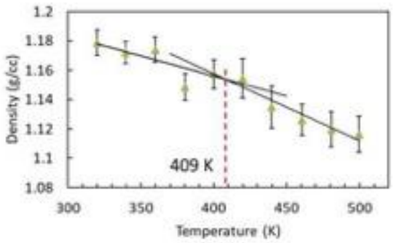




- Mechanical properties
  - Moduli, CTE, Tg, stress-strain, yield point
  - ReaxFF: Degradation rates & mechanisms
  - Heat transport (T-NEMD)



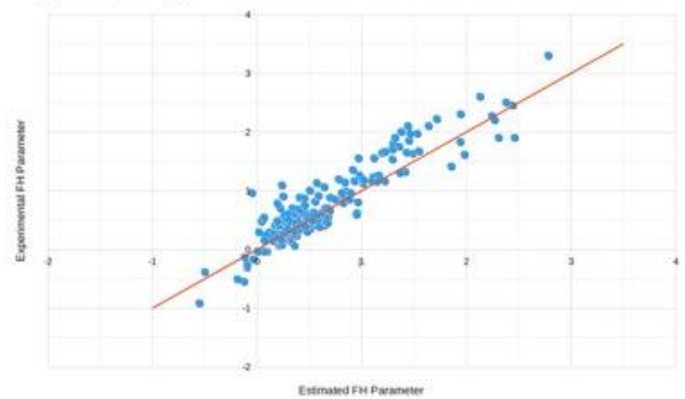




- Solubility and related
  - COSMO-RS, QSPR

$N_{p/s}$ – Number of moles of polymer / solvent
$\phi_{p/s}$ – Volume fraction of polymer / solvent
χ_{ps} – Flory – Huggins Parameter

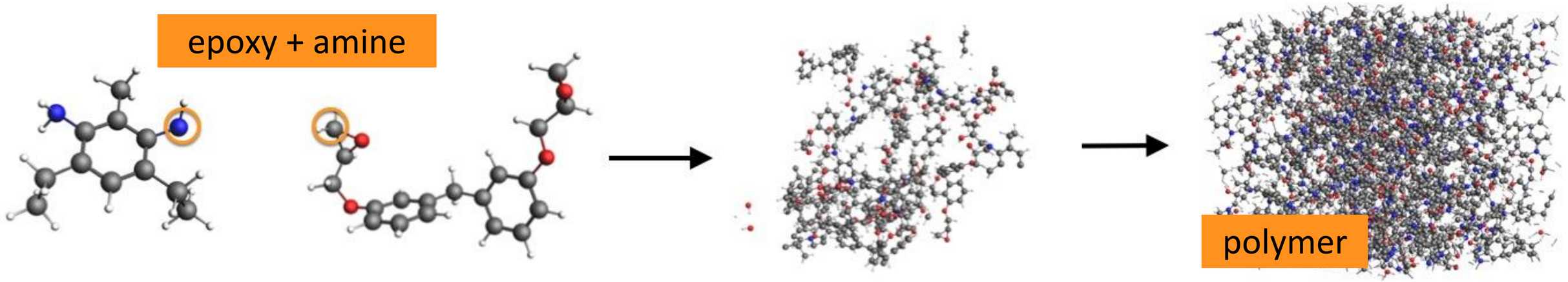
$$\frac{\Delta G_{mix}}{RT} = N_p \ln(\phi_p) + N_s \ln(\phi_s) + N_s \phi_p \chi_{ps}$$

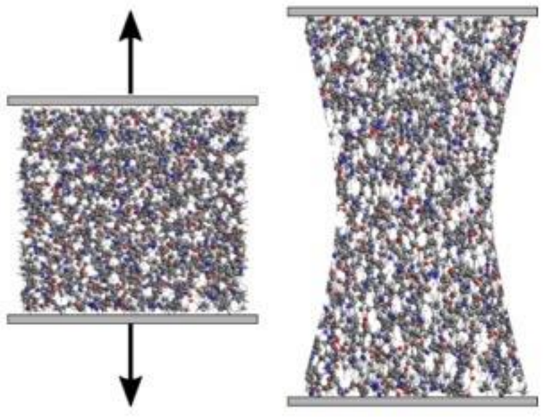


- (non-linear) optical properties, charge mobility
  - ADF & BAND

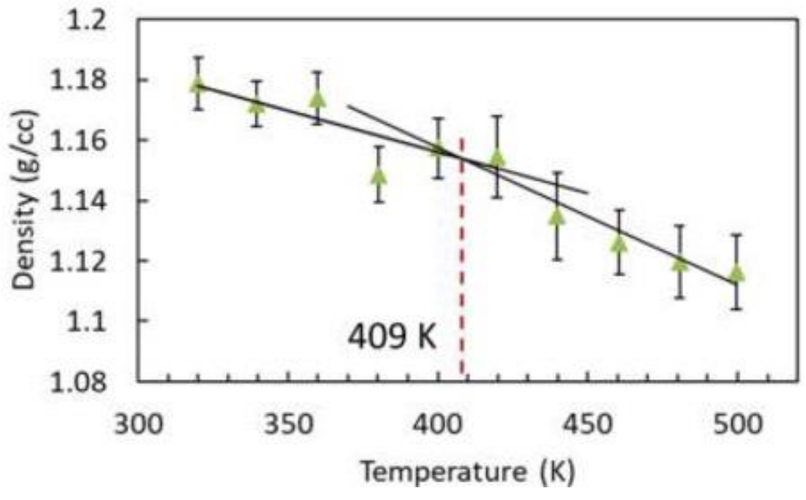
Epoxy polymers: structure & properties

- Understand & predict how cross-linking effects mechanical properties
  - Exp = slow: minutes to hours to reach ~80% cross-linking
  - ReaxFF: simulate few ns => accelerate kinetics to get highly xlinked structures





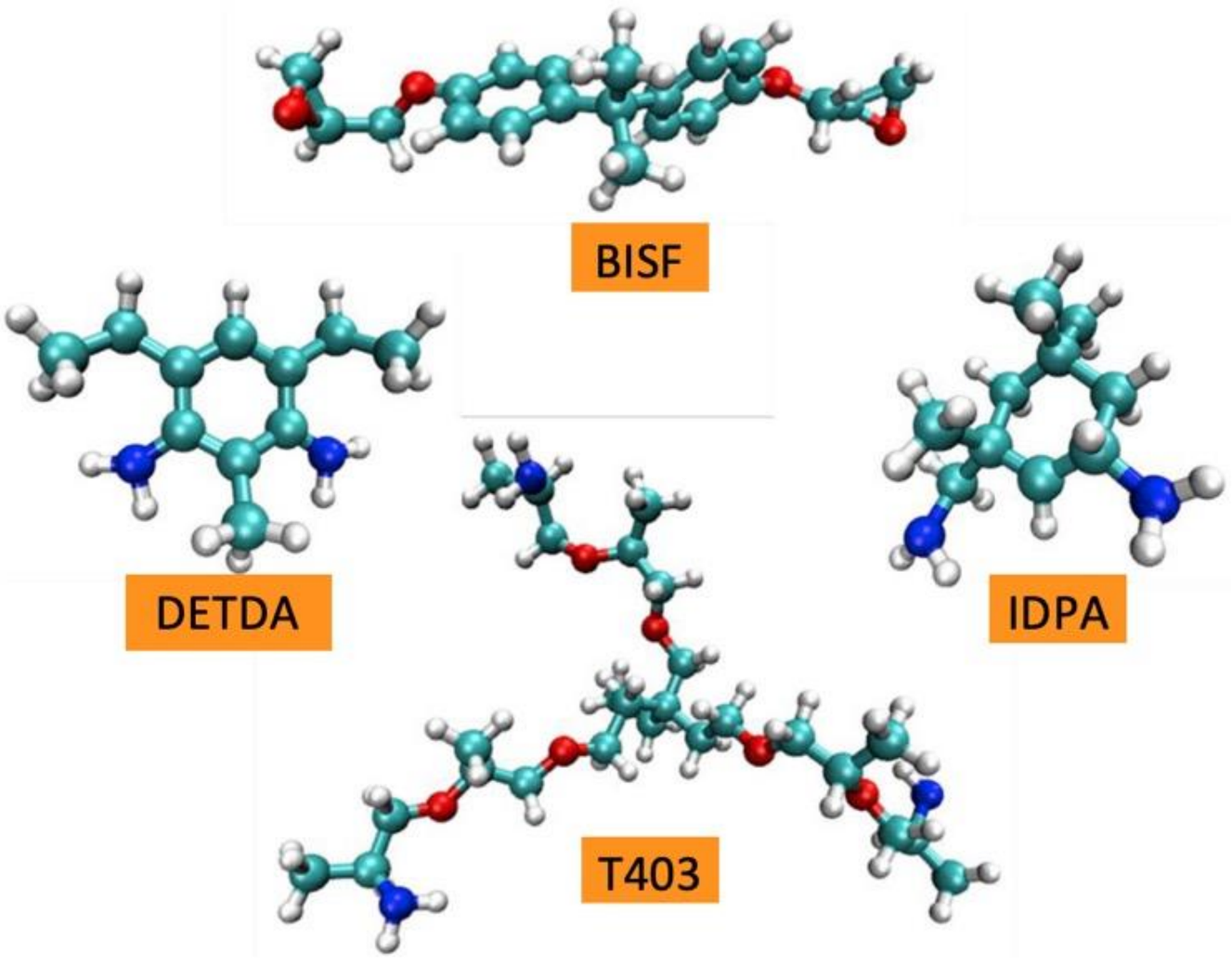
Modulus, yield point
J. Polym. Sci. B 2018, 56, 255

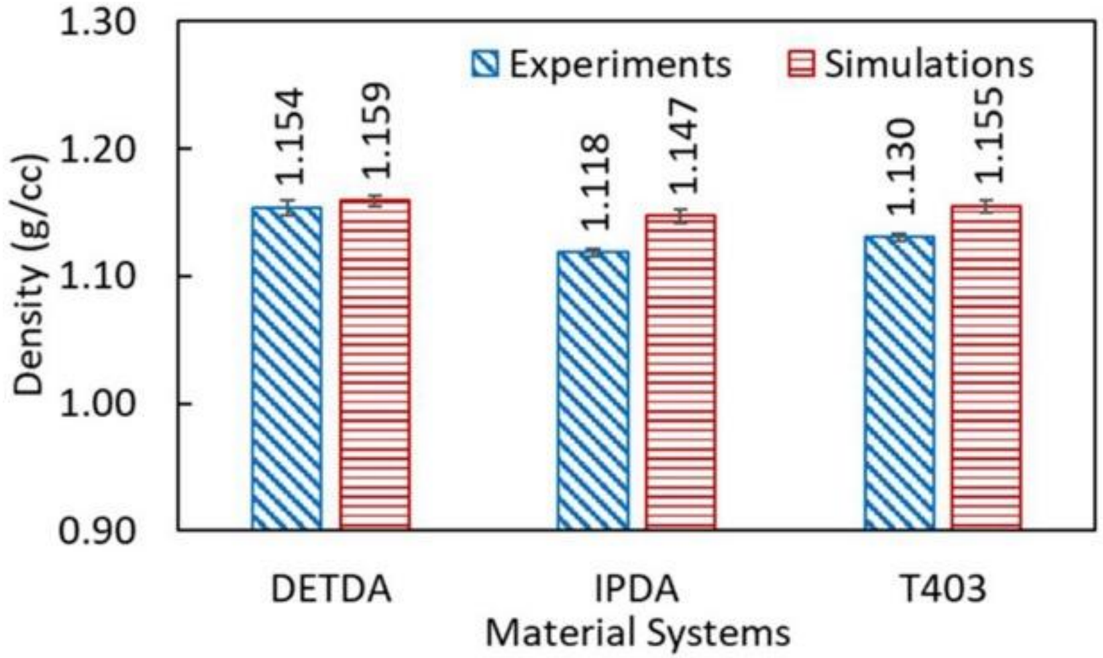


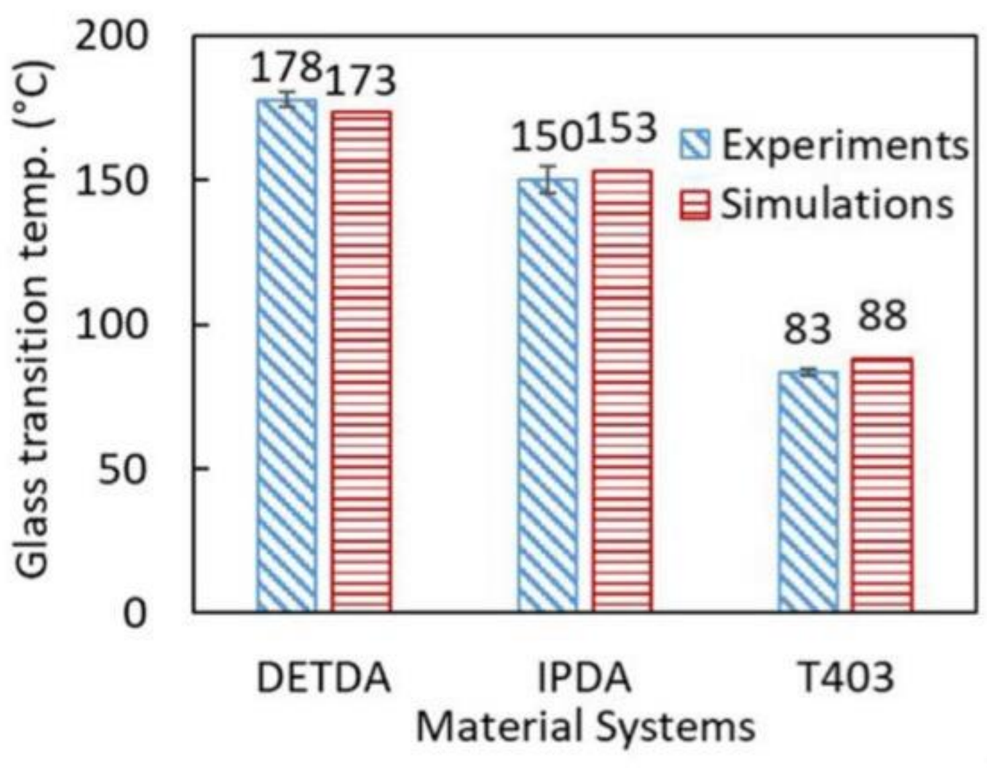
glass transition T_g

Properties of cross-linked epoxy polymers

- Good predictions: densities & T_g
- Aliphatic amine => lower T_g



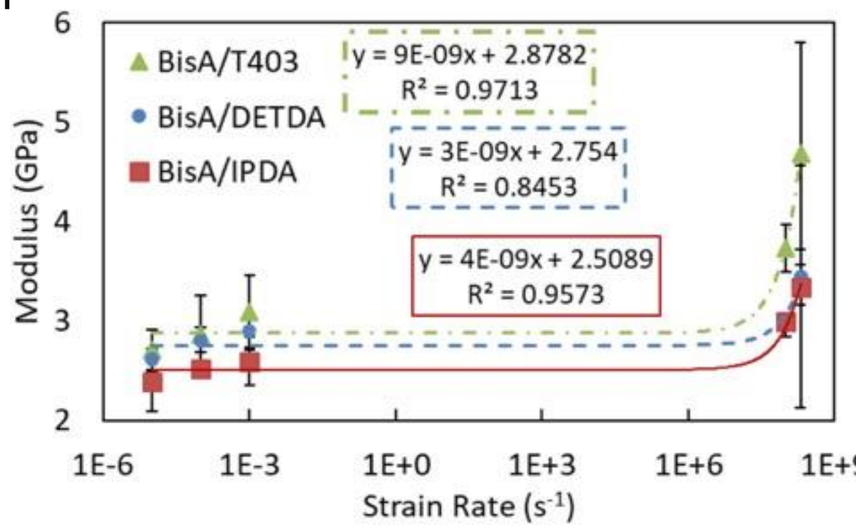


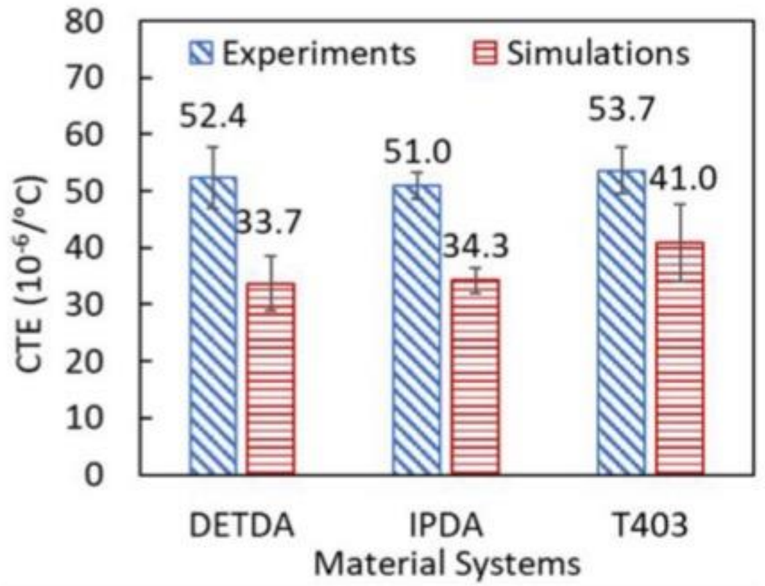


[Polymer 158, 354 (2018)](#)

Properties of cross-linked epoxy polymers

- Coefficients of thermal expansion too low
  - Reparameterize ReaxFF?
- Modulus: good linear fit (calc = high strain)
  - bulk stress tensors = faster
    - ReaxFF, DFTB





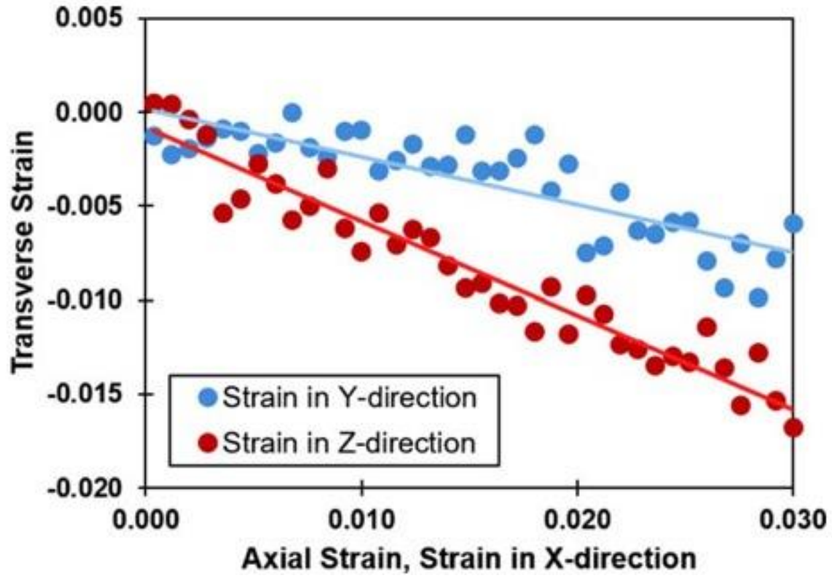
[Polymer 158, 354 (2018)](#)

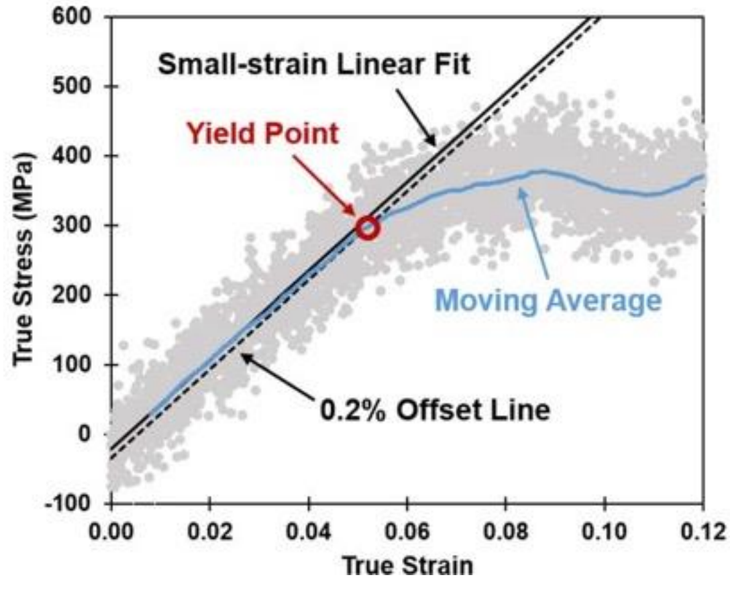
From Stress-Strain:

- Yield point(s)
- Strain ratios

Odegard group

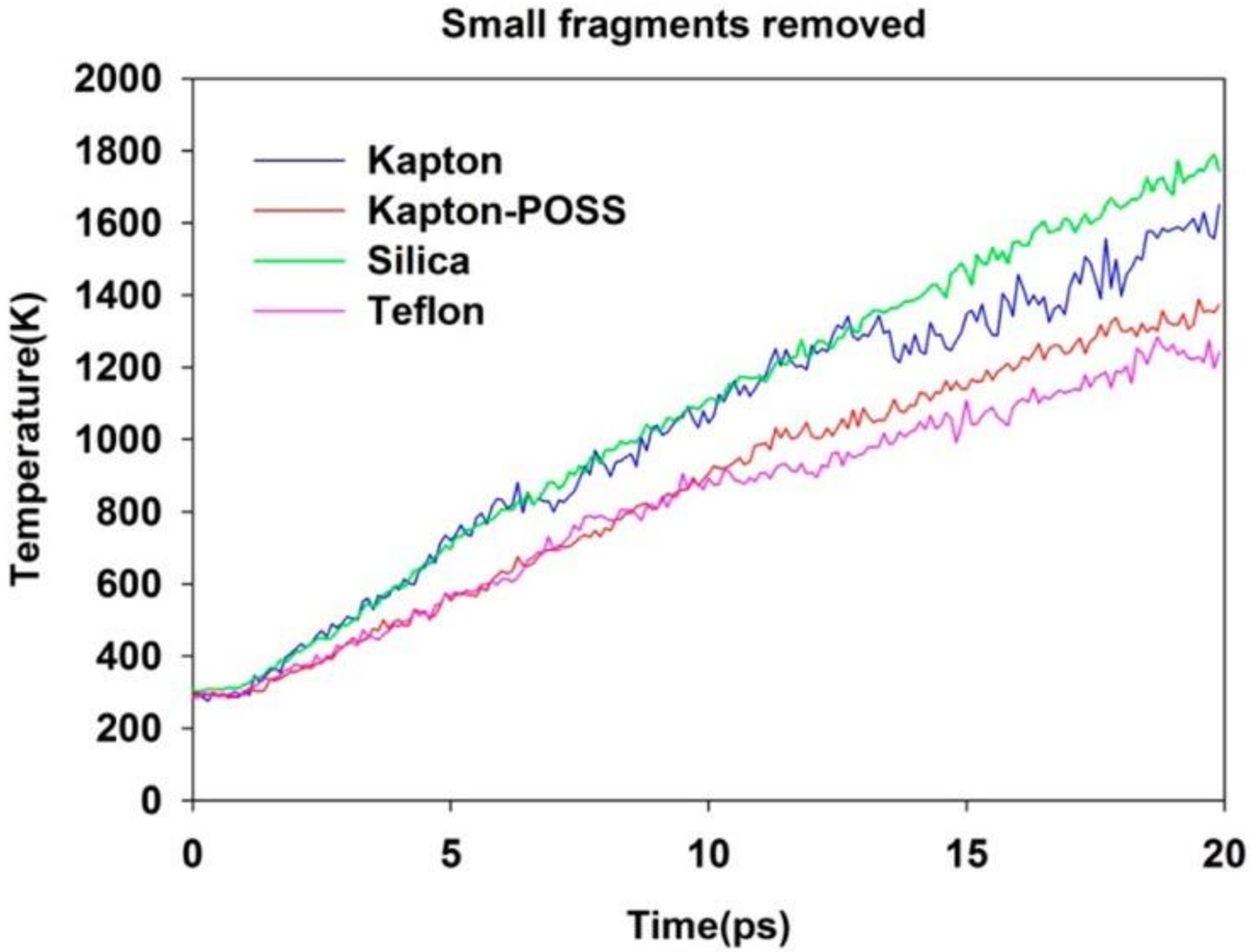
[J. Polym. Sci. B, 56, 255-264 (2018)](#)

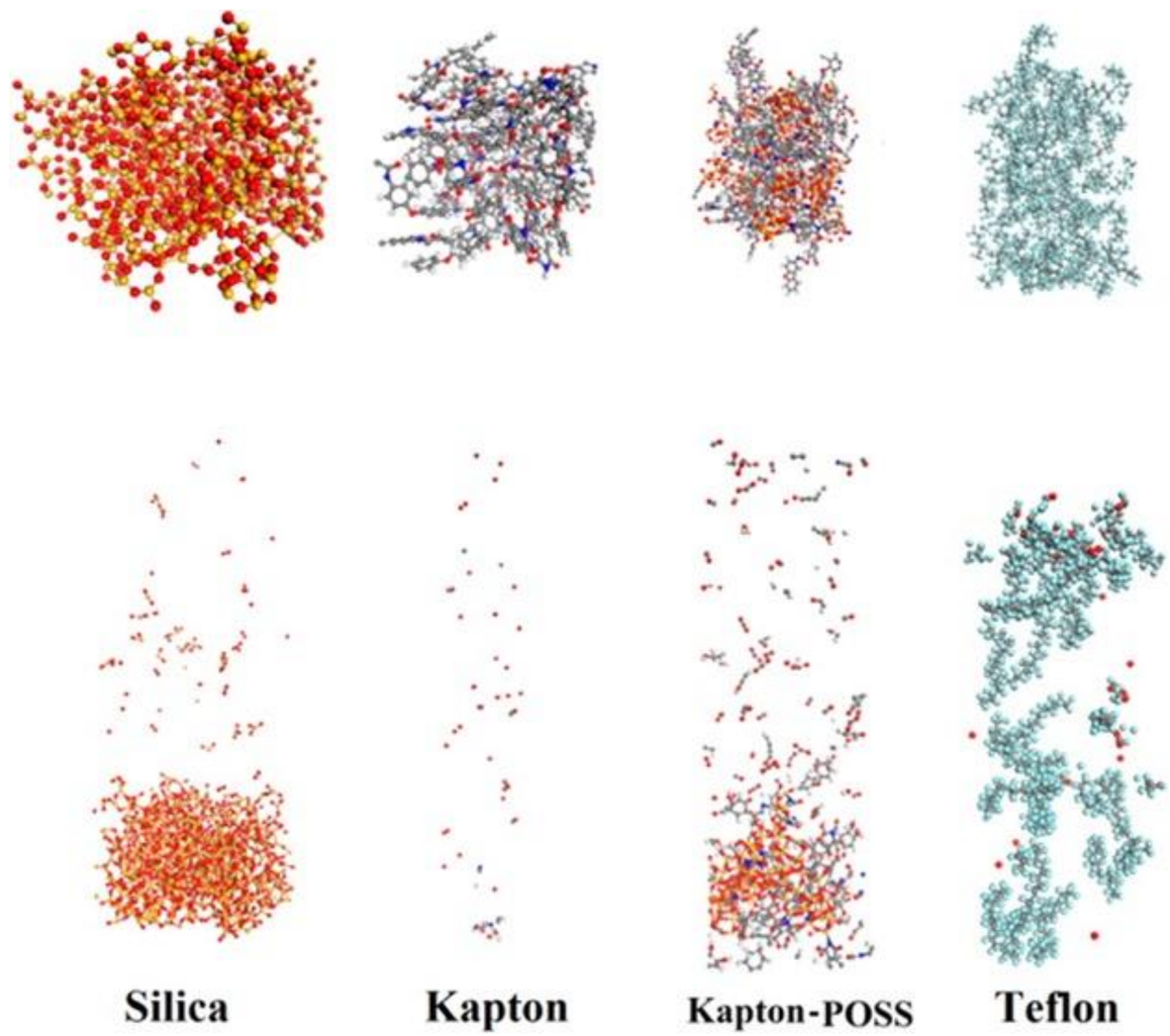




Degradation of polymers

- Atomic Oxygen bombardment studying low earth orbit conditions
- Silica is high initial resilience, Teflon lowest erosion rate
  - Good heat transfer properties can help; Kapton can be stabilized with silica.



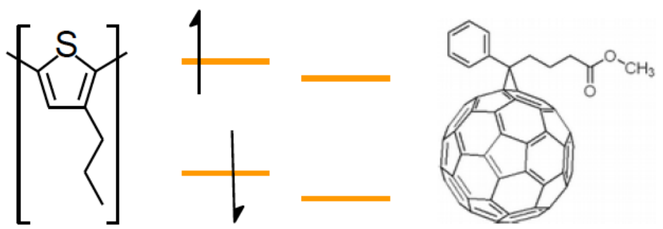


J. Phys. Chem. A, 2014, (118), 2780

Polymer mixture design with COSMO-RS

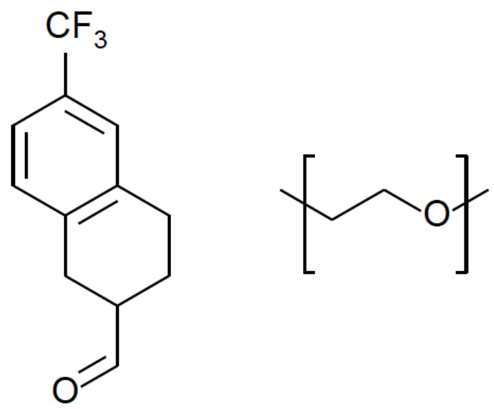
- COSMO-RS: mixture thermodynamics
  - Liquid-activity coefficient
  - Fit to experimental data (predictability outside fit)
  - Pseudo-chemical potential from quantum mechanics (surface charges)
- Existing design approaches focus on property targeting (QSPR)
- Mixing => requires free energies, activities

Organic electronics



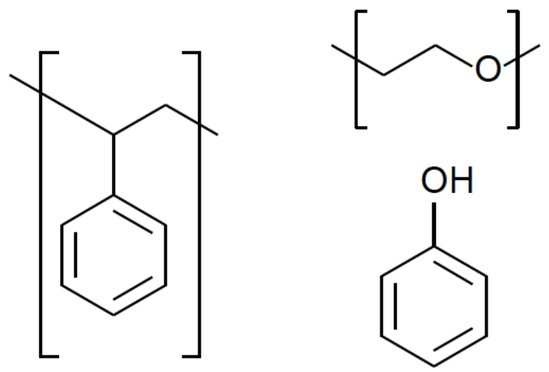
- Phase stability
- Polymeric batteries

Drug Solubility



- Poorly water-soluble drugs
- Bioavailability

Polymer/Solvent-Polymer interactions



- Flory-Huggins parameters
- Swelling, solubility of polymer blends, etc.

How we help you develop new materials

- Advanced computational chemistry software
  - Amsterdam Modeling Suite: from DFT to reactive potentials
  - Easy to use, powerful methods

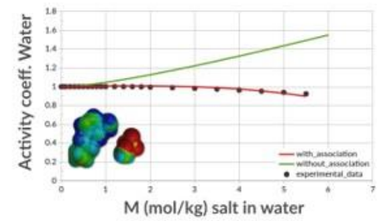
- Integrating multi-scale methods
  - ReaxPro: kinetics, fluid dynamics for catalysis
  - Simbeyond: atomistic-to-device scale OLED modeling
  - Wasatch: battery & fuel cell modeling

- Integrating Machine Learning methods

- Expert scientists and software developers
  - Decades of expertise in pragmatic software development
  - Support & development to help your RD&I

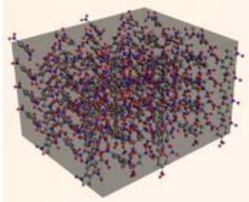
Amsterdam Modeling Suite

- ADF: powerful molecular DFT
  - Reactivity, spectroscopy
- BAND: periodic DFT, QE & VASP interface
  - (2D) Materials, spectroscopy, analysis
- DFTB & MOPAC: fast electronic structure
- ReaxFF: Reactive MD complex systems
- MLPotential
  - Backends SchNetPack, sGDML, PiNN, TorchANI
- COSMO-RS: fluid thermodynamics
  - VLE, LLE, logP, solubility
- AMSdriver: PES exploration, MD, MC
  - Hybrid: multi-layer, QM/MM, QM/QM'
- Integrated GUI, PLAMS: python scripting
- Interface with multi-scale and ML methods

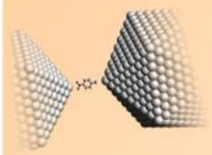


Continuum

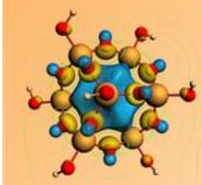
AMS driver GUI PLAMS



Materials



Nano



Atomistic

COSMO-RS
Fluid Thermodynamics & Property Estimation

ReaxFF
Reactive Force Field

MLPotential
Machine Learning Potentials

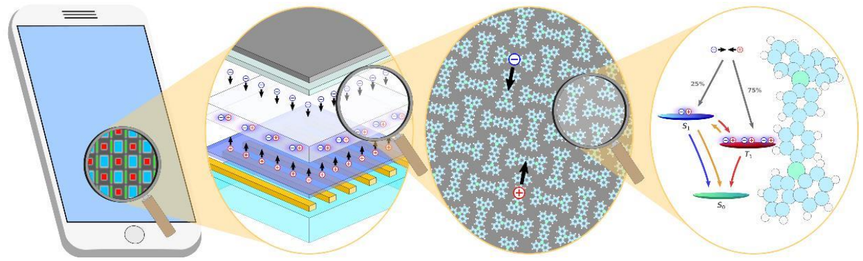
DFTB & MOPAC
Fast approximate DFT Semiempirical

BAND
Periodic DFT

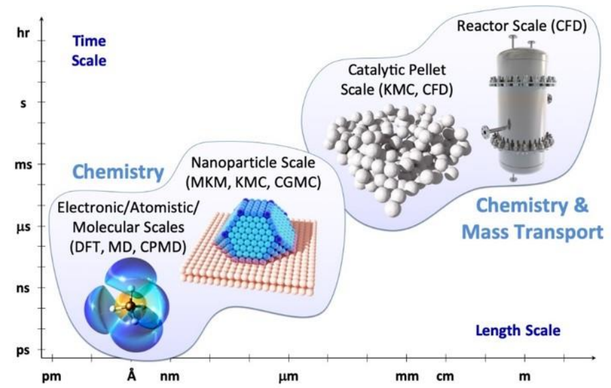
ADF
Molecular DFT

Relevant materials and applications

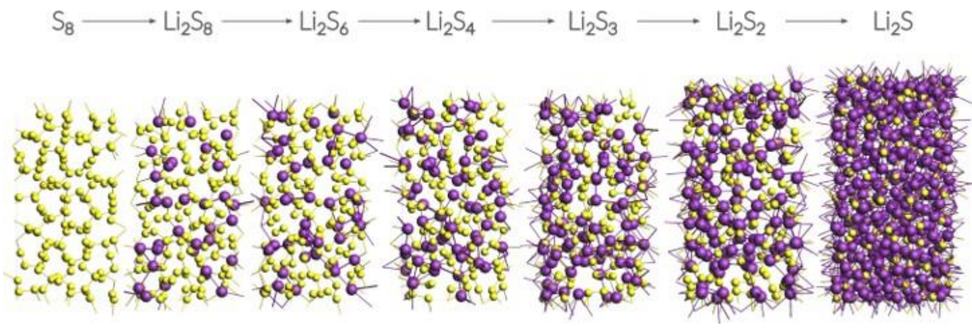
- OLEDs, OFETs, OPVs
  - Charge & exciton mobility
  - Absorption, luminescence
  - Multi-scale device modeling



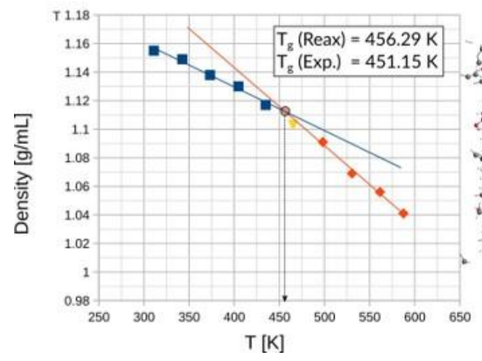
- Catalysis
  - Map reaction pathways
  - Optimize TOF
  - Atomistic-to-plant multi-scale

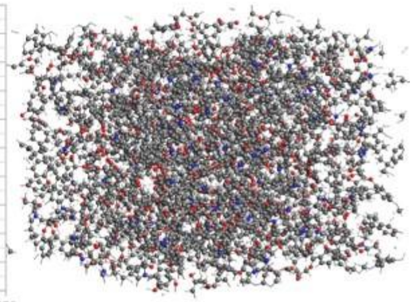


- Batteries
  - Electrolyte solubility
  - Degradation
  - (Dis)charge processes, mobility



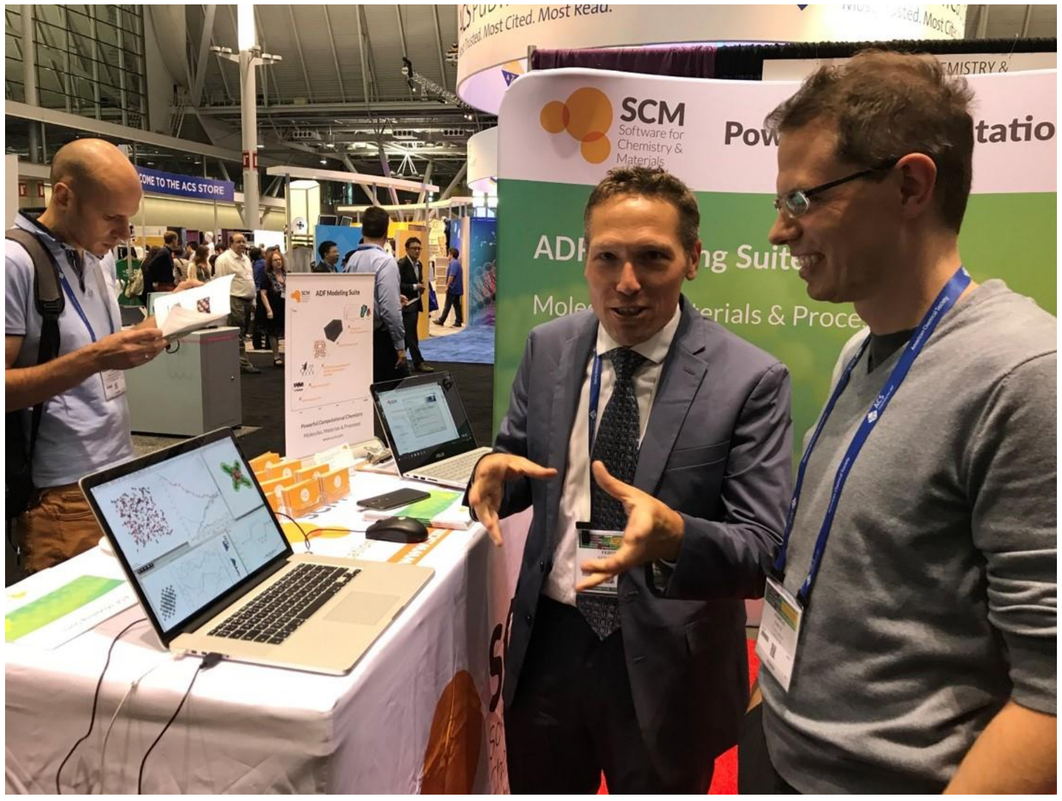
- Polymers
  - Mechanical: CTE, Tg, yield point
  - Optical: n_i, loss, κ
  - Reactivity: formation, degradation





Discuss your research challenge!

Which materials would you like to develop faster?
What are the key properties?



We love to hear from you!
goumans@scm.com
www.scm.com