Modeling molecular properties for organic electronics

OLED emitters, charge mobilities, and other properties

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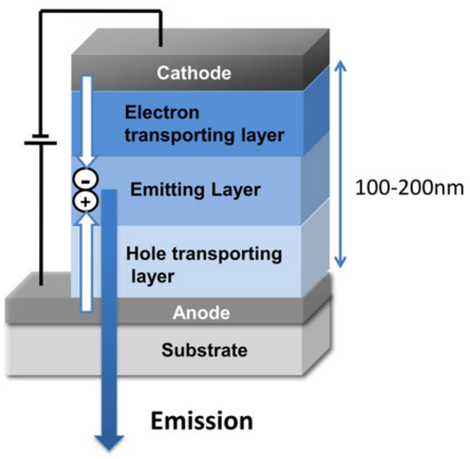
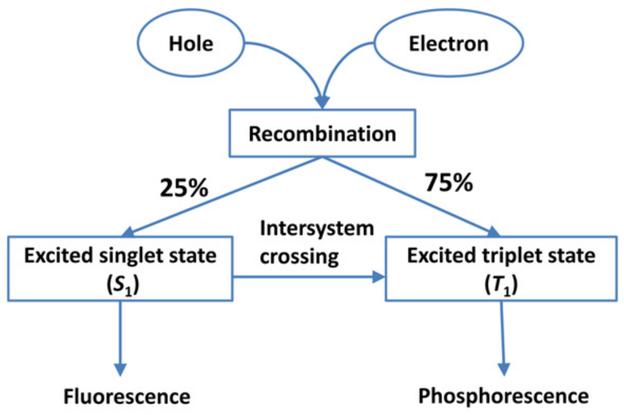
Phosphorescent emitters

Organic light-emitting diodes (OLEDs) convert electricity into light, by emitting from excited states (excitons) formed upon recombination of charges. Phosphorescent OLEDs improve the conversion efficiency by harvesting all excitons as triplets which subsequently phosphoresce.



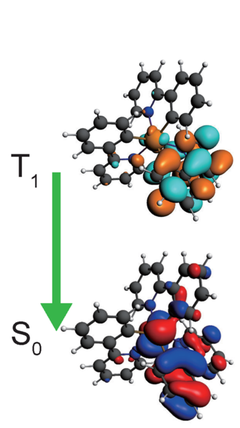


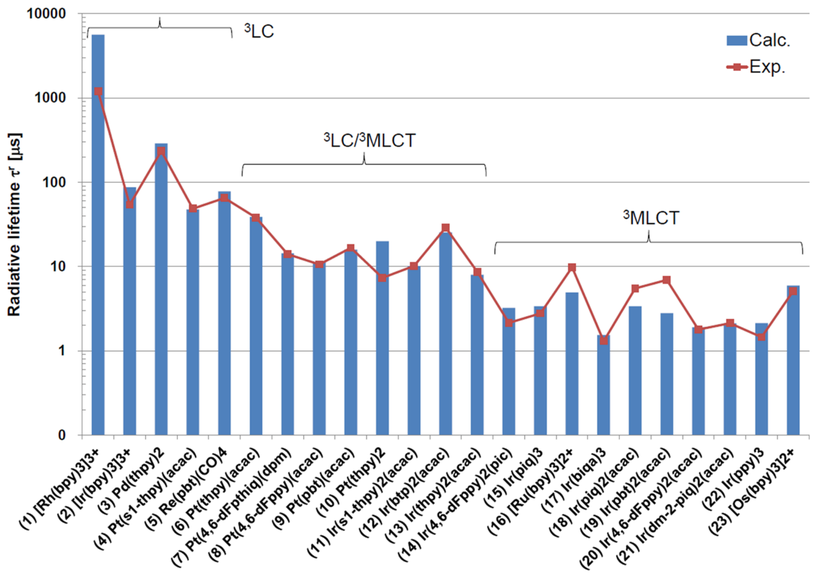
Y. Suzuri et al., Sci. Technol. Adv. Mater. 15 (2014) 054202.

OLED efficiency can be optimized by maximizing intersystem crossing and phosphorescence rates. This in turn is effectuated by transition metal complexes with large spin-orbit coupling, which mixes singlet and triplet states.

Virtual screening OLED emitters

Novel OLED emitters can be screened and optimized through modern computational chemistry techniques. Spin-orbit coupling TDDFT in ADF reliably predicts phosphorescent lifetimes and zero-field splitting (ZFS) across a diverse range or transition metal complexes.





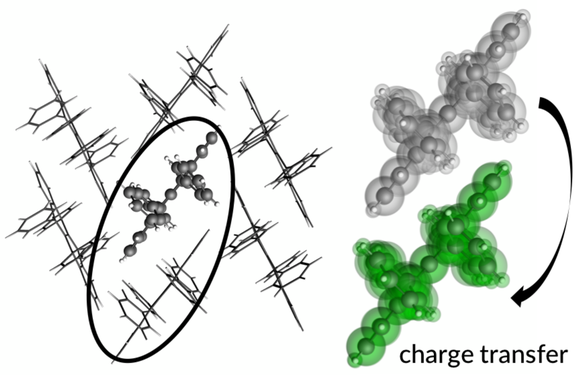
K. Mori et al., Phys. Chem. Phys. Chem.16, 14523 (2014)

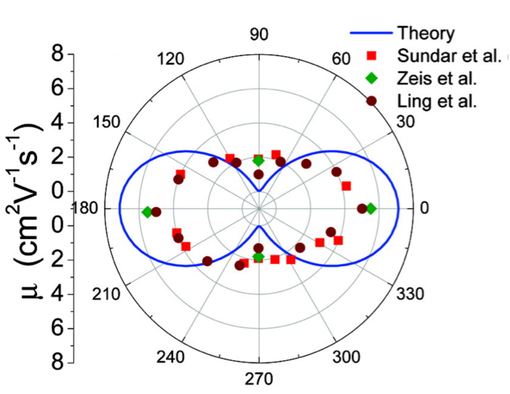
See also Younker and Dobbs, J. Phys. Chem. C, 117, 25714-25723 (2013) for a pragmatic screening approach.

Rational design of organic electronics with modern computational chemistry, giving a handle on several important material properties at the molecular level.

Charge carrier mobility

Hole and electron mobilities are also important properties for optimizing organic electronic devices (OLEDs, OFETs, OPVs). The charge transfer integral approach in ADF is an efficient way to screen hopping rates, from which charge mobilities magnitudes and anisotropy can be calculated.





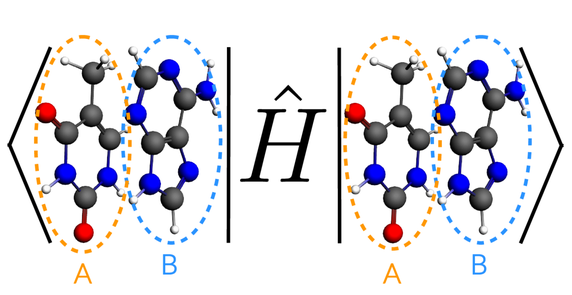
S.-H. Wen et al., J. Phys. Chem. B 113, 8813-8819 (2009)

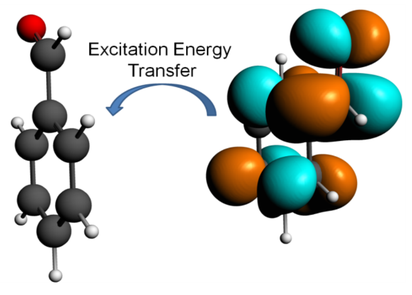
A more sophisticated, all electron method to calculate electronic couplings is available via the frozen-density embedding (FDE) formalism from the Neugebauer & Pavanello groups. Environment effects (polarization) can be includes and charges and excitons can be localized.

In the same *ansatz*, charge carrier generation from excitons can be modeled (J. Chem. Phys. 140, 164103 (2014).

Exciton coupling & quenching

Besides charge generation and mobility, the FDE approach in principle gives access to other properties of interest for organic electronics: exciton coupling, singlet fission, exciton-polaron coupling, exciton-exciton quenching, etc.





König et al., J. Chem. Phys. 138, 034104 (2013)

Intersystem crossing, TADF

Triplet to singlet intersystem crossing in organometallic dopants is also dominated by spin-orbit coupling and can thus be assessed with ADF, e.g. Phys. Chem. Chem. Phys. **16**, 26184-26192 (2014).

To optimize reverse intersystem crossing, important for thermally activated delayed fluorescence (TADF), the analysis tools in ADF can be used to scrutinize the charge transfer excitations and minimize the S-T gap.

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