Emission Color Pureness and Efficiency Regulation in Organic Chromophores

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Luminescent conjugated organic chromophores have found immense interest in current materials research, and rapid progress has been seen over the past years. In any case, the quest for sustainable research demands pre-synthesis tailor-made targeted design beyond experimental (and computational) trial-and-error strategies. This can only be achieved by a thorough understanding of the underlying photophysical process combined with spectroscopic and computational techniques. In this spirit, the seminar will focus on key parameters of emissive organic materials, being (i) luminescence efficiency and (ii) color purity, being both crucial in particular for OLED research.

Luminescence efficiency is decided by the competition of radiative vs. nonradiative processes. Nonradiative decay via internal conversion (IC) is frequently tackled via 'Fermi's Golden Rule' (FGR).[1] However, in particular for systems with very effective IC, FGR may break down both in a quantitative and qualitative manner. This was especially shown for compound families which establish an 'inverted energy gap law',[2] sharply contrasting the prediction of FGR. Instead, this has to be treated via conical intersections (CIs). In the solid state, IC becomes often a minor pathway, as the access to the CI often involves large amplitude motions,[2] giving rise to 'Solid State Luminescence Enhancement' (SLE).[1,2a] On the other hand, examples of active CIs in solid state samples have been identified, due to the absence of large amplitude motions on the path to the CI,[3,4] so that fluorescence quenching persists in molecular solids.

Color purity, measured by the effective spectral width,[5] can be conveniently predicted within commercial quantum chemistry program packages; however; while this generates quite accurate numbers, it does not provide understanding. We will show that such understanding – 'beyond numbers' – can be achieved at a simple conceptual basis using resonance theory and MO topology consideration; this allows for targeted 'paper and pencil' molecular design of color pure emitters, ranging from the UV to blue region[5] to the deep red/NIR.[6]

References

[1] For a recent review on this matter, see J. Gierschner et al, Adv. Opt. Mater. **2021**, 9, 2002251.

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[4] J.-M. Heo et al, Nat. Commun. **2025**, 15, 5560.

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