Investigation into the synthesis and technological application of near-infrared emitting excited dimers (excimers)

Introduction and Context

Interest in organic-light emitting diodes (OLEDs) has grown rapidly over the past decade. By incorporating phosphorescent metal complexes, the maximum efficiency of 25% for fluorescent OLEDs can potentially be increased to 100%. Near-infrared (NIR) light of wavelength 700 – 1400 nm is technologically important, with applications in telecommunications, night vision, photodynamic therapy,[5] and state-of-the-art finger-print technology.[2] However, no efficient NIR OLEDs are currently available! Large multinational companies are consequently interested in developing such materials; *e.g.*, Samsung are already supporting aspects of this science at Durham University.

The research question

A number of molecular phenomena conspire to compromise the efficiency of such low-energy emitters. Electronic energy is more readily dissipated into molecular vibrations – often known as the energy gap law. Another problem in OLEDs is that upto 75% of the energy goes into forming triplet excited states – ones in which two electrons have parallel spins – as opposed to singlet states, where the spins are opposed. Normally, quantum mechanical rules mean that only the singlet states can emit light. Heavy elements like iridium are currently added to the materials used in many OLED screens in order to side-step these quantum restrictions. But as one moves towards the red and NIR, the effect of such metals falls off.

The research project will contribute to the development of a hitherto little explored strategy for targeting deep red and NIR emission. The strategy will involve the use of metal-containing *excimers* (excited dimers). They were first discovered in the 1960s when the fluorescence of planar organic molecules like pyrene were studied. An excited state is formed that spans two molecules and is lower in energy than the isolated molecules – in other words, the emission moves towards the red region of the spectrum. There has been little work on analogues containing metals,[7] and the project will aim to redress this and consider how metal excimers can be further used to obtain NIR-emitting OLEDs.

The objectives of the research will be:

1. To prepare up to three new, planar molecules containing platinum bound to organic units by at least one Pt–C bond.
2. To study the light absorption and light emitting properties of these new molecular materials in solution, and detect excimer formation
3. To examine the luminescence of the best performing materials when embedded in OLED host materials, or as neat films.
4. To use selected materials to construct OLED devices and test their effficiency with regard to deep red and NIR emission with Durham Physics

Methodology

The initial part of the project will require the synthesis of new suitable ligands to be tested for near-infrared (NIR) emittance. The structure of ligands I will be synthesising involve two adjacent pyridyl rings (a ring of five carbons and one nitrogen atom) with one ring bonded to an electron withdrawing group such as fluorine, and the other ring bonded to an electron donating group such as an ester. Synthesis of these molecules will be achieved using contemporary methods including metal-catalysed cross-coupling reactions. The purified molecules will be treated with platinum salts to evolve compounds containing the Pt-C bond. To evaluate the photophysical properties of the new platinum-containing compounds they will need to be sufficiently pure. Devising experimental methods to increase purity at this stage will be vital. To test the final purity of the platinum-containing compounds I will use nuclear magnetic resonance spectroscopy, and mass spectroscopy with elemental analysis which I will have access to within the chemistry department.

The next part of the project will involve testing for excimer formation from the synthesised platinum complexes. To do this the distribution of colours (spectrum) emitted from the compounds in solution will be examined at different concentrations. If excimer formation occurs, the proportion of light emitted in the red and NIR region will increase as concentration increases. This is because, at higher concentrations, the probability of two molecules coming together to form excimers increases. Other photophysical properties, such as brightness to give the quantum yield, will be determined using equipment in the Chemistry Department.

After identifying molecules in solution that form excimers or high NIR emission efficiency, they will be examined in the solid state – in either host materials or neat films – since these are the conditions that apply to OLEDs. Ideally a material will be obtained that, under these conditions, shows uniquely excimer-like emission in the NIR. This material can then be tested as the emitter material in an OLED in the Physics Department, using fabrication methods such as vacuum sublimation or solution processing.

References

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