Project:

HyperOLED

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"Development of high-performance, hyperfluorescence OLEDs for use in display applications and solid state lighting"

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D1.6 Comparison of measured and calculated emission characteristics of emissive core structures

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Dissemination Level		
PU	Public	X
PP	Restricted to other program participants (including the EC Services)	
RE	Restricted to a group specified by the consortium (including the EC Services)	
CO	Confidential, only for members of the consortium (including the EC)	

The H2020 HyperOLED project is a three-year EC funded project entitled "Development of high-performance, hyperfluorescence OLEDs for use in display applications and solid state lighting". The project will run from January 2017 to December 2019.

The overall goal of the HyperOLED project is to develop materials and matching device architectures for high performance, hyperfluorescence organic light emitting diodes (OLEDs) for use in display applications and solid state lighting. The innovative OLEDs will be realised by combining thermally activated delayed fluorescence (TADF) molecular hosts with novel shielded fluorescence emitters, targeting saturated blue emission of very high efficiency, especially at high-brightness levels.

Further efficiency gains will be achieved through molecular alignment to enhance light outcoupling from the hyperfluorescence OLEDs. Using shielded emitters will enable simpler device structures to be used, keeping drive voltages low to be compatible with low voltage CMOS backplane electronics. This will enable demonstration of the concept's feasibility for high-brightness, full-colour OLED microdisplays as one application example.

To develop the hyperfluorescence OLEDs, the following scientific and technical objectives will be targeted:

- Objective 1: Develop shielded emitters

- Objective 2: Develop TADF hosts

- Objective 3: Photo-physically characterise the shielded emitters and TADF hosts

- Objective 4: Anisotropic molecular orientation for enhanced performance

- Objective 5: Design and test prototype hyperfluorescence OLEDs

- Objective 6: Fabricate and evaluate demonstration hyperfluorescence microdisplays

To show the project's overall goal has been achieved, multiple blue and white stack unit prototypes (2 x 2 mm² on 30x30mm glass substrates with ITO) will be integrated into a high-brightness microdisplay demonstrator (based on MICROOLED's 0.38'' WVGA CMOS backplane) and tested that demonstrate significant improvements in functionality, performance, manufacturability and reliability.

1. Motivation

In today's commercially available organic light emitting diodes (OLEDs), so-called small organic molecules are used for fabrication. This broad class of materials contains a virtually infinite number of different chemical compounds, resulting in difficulties to choose the best performing compounds by simple trial and error testing. Apart from experience and other considerations, computational methods have thus become more and more important in the last years in this respect. It is thus no surprise that the HyperOLED project also relies on these methods for the choice of new materials.

One important material parameter that has to be considered is the emission colour. We are targeting blue emission and therefore, we have to choose materials accordingly. A lot of known chemical structures emit in the blue region of the spectrum and are suitable for use in OLEDs. However, the very specific requirements of the HyperOLED project imply that molecules traditionally used in OLEDs cannot be employed. The project consortium thus needs to look for new chemical structures and assess existing ones regarding their usability. Computational chemistry is a good approach to help us in this regard. By considering the results from simulations, we can preselect the most promising targets which increases development speed and leads to an efficient use of resources. To make the predictions as accurate as possible, we calibrate the computer simulations based on measurement results as described in the following.

2. Measurements

A widely used method to obtain the emission colour of a material is photoluminescence spectroscopy (PL, also called fluorescence spectroscopy). In such an experiment, the sample under study is excited by light. The energy absorbed in this process can be emitted by the material as light with lower energy. The spectrometer records this light and generates an emission spectrum. In our experiments, we dissolved a small amount of material in the solvent toluene. This solution is filled into a quartz cuvette and measured in the spectrometer. An example of a measured spectrum is shown in the following *Figure 1*.
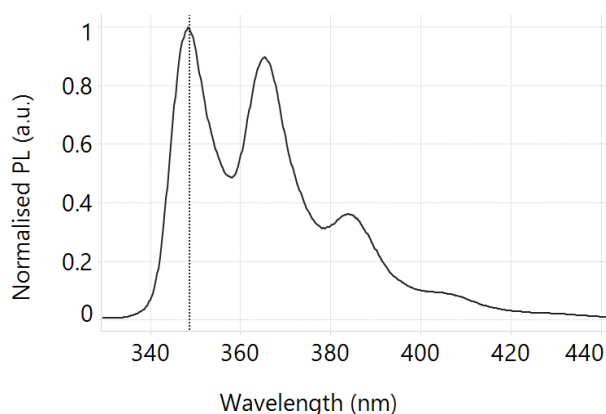

Figure 1: Example of a measured PL spectrum. The dotted line shows the position of the first peak.

The emission colour can be calculated from the recorded emission spectrum, but for the comparison of the measurements and calculations, we use the position of the first peak in the spectrum, which is around 350 nm in the figure above.

3. Calculations

To preselect material candidates, we count on simplified calculation methods. On the one hand, this approach has the advantage of speeding up the process by reducing computation time. On the other hand, simplifications lead to errors and less accuracy which has to be taken into account.

The most significant assumption that we make is that we calculate the process of *absorption* of light and not that of light *emission*. The reason is that it is very difficult to calculate the geometry of a small organic molecule that was excited by light. On the other hand, the geometry of the molecule in the ground (not excited) state is quite easy to calculate. Now the emission process starts from the excited state while the absorption starts from the ground state, making it much easier to calculate. This assumption appears quite odd at first sight because we want to calculate the emission characteristics. However, absorption and emission are related processes and for the molecules we consider, the offset between absorption and emission does not vary too much between molecules so that this assumption is justified. Nevertheless, it results in an error that we have to take into account.

In technical terms, we first optimise the molecular ground state geometry at the B3PW91/6-31G(d) level of theory. To obtain the absorption energy, we carry out TD-DFT (time-dependent density functional theory) calculations of vertical singlet excitation energies using the same method (i.e., B3PW91/6-31G(d)).

4. Calibration

For a number of compounds, we carried out the PL measurement as well as the calculations as described in the last two sections. The results of this are plotted against each other which gives the graph shown in *Figure 2*.
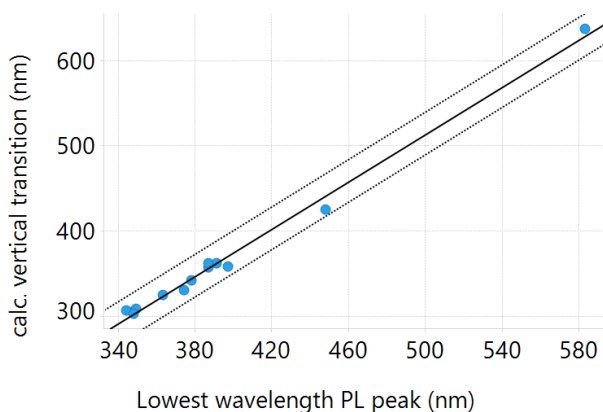

Figure 2: Calculated vertical transition vs measured position of the lowest wavelength peak from the PL spectrum for a number of compounds. A straight line can be fitted to the data with an R² of 0.992 (solid line). The dotted lines show the fit +/-25 nm which gives a rough estimate of the expected deviation between calculation and measurement.

A straight line can be fitted through the points (shown as solid line in the graph). The deviation of the calculations from the fitted line gives a rough estimate of the error in our prediction which is indicated by the dotted lines.

We can now carry out calculations for unknown materials which we think might be worth investigating and use the fit we obtained to estimate the emission colour. Materials which lie outside the required wavelength range are not considered for further analysis. In this sense, the calculations can be regarded as a "filter", not a prediction tool: We can predict what should *not* be done rather than exactly say what we should do.

5. Conclusions

We have presented methods to measure and calculate the emission characteristics of fluorescent materials. By comparing experimental measurements and computer simulation results for a number of compounds, we can calibrate our calculations to obtain estimated emission colours of unknown compounds purely by computer simulations. This approach significantly helps to improve the selection of emitting materials in the hyperfluorescent OLEDs that are developed in the HyperOLED project. Valuable resources are saved and the development speed is increased.