Periodic Reporting for period 2 - PHEBE (New paradigms for high efficiency blue emitters for white OLEDs)

**Reporting period:** 2016-02-01 to 2017-01-31

**Summary of the context and overall objectives of the project**

The overall objective of the PHEBE project is to develop innovative, high-efficiency, blue emitters for white OLEDs, which will create a major breakthrough in the cost performance of OLED lighting. To produce the innovative blue emitters, two new types of molecular systems – without rare earth complexes - will be investigated:

- intramolecular charge transfer systems that enable thermally activated delayed fluorescence (ICT-TADF)
- intermolecular exciplex charge transfer systems that enable thermally activated delayed fluorescence (Exciplex-TADF)

In order to develop the ICT-TADF and Exciplex-TADF based emitters, the following scientific and technical objectives will be targeted:

- **Objective 1:** Screen potential ICT-TADF and Exciplex-TADF compounds with theoretical models
- **Objective 2:** Synthesise the most promising ICT-TADF and Exciplex-TADF model compounds
- **Objective 3:** Characterise and select the best ICT-TADF and Exciplex-TADF synthesised compounds
- **Objective 4:** Design white stack units employing the selected TADF based emitter and block materials
- **Objective 5:** Design close-to-production OLED lighting panel demonstrators

To show the project’s overall objective has been achieved, white stack tandem units (2 x 2 cm2 with 90 nm ITO) and OLED lighting panel demonstrators (e.g. 25 cm2 circular panels) - based on the new blue emitters – will be produced and tested that meet the performance targets indicated in the H2020 call ICT 29 – 2014.

**Work performed from the beginning of the project to the end of the period covered by the report and main results achieved so far**

The work performed and main results achieved by the PHEBE project from the start until the end of Period 2 have been as follows:

**WP1 Modelling**

- TUD has implemented a workflow model to screen possible TADF emitters.
- Novaled has designed and provided over 80 molecules for modelling.
- TUD has developed a tool for modelling molecular pairs and a scheme to evaluate CT processes.
- TUD has developed a computational scheme for the analysis of CT transitions at donor-acceptor interfaces in bulk
heterojunctions of photovoltaic cells.
• TUD has developed a programme for calculating Huang-Rhys factors along each vibrational normal mode of the synthesized material classes.

• Deliverable D1.1 “Table with state-of-the-art TADF emitters and their properties collated” was submitted on schedule.
• Deliverable D1.2 “Report on initial model to predict TADF PLQY” was submitted on schedule.
• Deliverable D1.3 “Initial report on molecular control of TADF” was submitted on schedule.

WP2 Synthesis
• KTU has synthesised and characterised a number of new exciplex forming derivatives containing 2-quinolone and quinoline moieties.
• KTU has synthesised and characterised a number of new ICT TADF material: dimethylxanthone containing derivatives, decafluorobihenyl containing derivatives and phenylcarbazoles
• Deliverable D2.1 “Midterm report on synthesis and chemical characterization of new ICT materials produced” was submitted with a small delay of a few months.
• Deliverable D2.2 “Midterm report on synthesis and chemical characterization of new exciplex-forming materials produced” was submitted on schedule.

WP3 Characterisation
• UDUR has photophysically characterised a series of donor-π bridge-acceptor (D-π-A) molecules. Although the molecules showed strong ICT character, the delayed fluorescence was found to occur by a triplet-triplet annihilation mechanism.
• TUD and UDUR have photophysically characterized the phenyl-carbazole, the trimer family, and a series of benzoate molecules. While the phenyl-carbazoles and the benzoates show significant TADF contribution, TADF is only weakly observed in the trimers.
• UDUR have identified three regimes for TADF based upon the spin-orbit charge transfer (SOCT) theory for reverse intersystem crossing (RISC).
• UDUR’s study into quenching in an optimised blue TADF device has shown that polaron quenching is not the largest issue for device performance currently. Electrometer emission in some of the hole injection layers and poor hole transport in the host layer seem to be some of the major reasons behind poor performance in the devices.
• UDUR has shown strong links between the anisotropy of the CT state and local triplet state in anisotropic TADF emitters. It is postulated that this is as a result of the vibronic-coupling mixing the states and thus sharing anisotropy.
• Deliverable D3.1 “Report on the effect of electric fields on TADF” was submitted on schedule.
• Deliverable D3.2 “Report on CT state-polaron interactions in TADF devices” was submitted with a small delay of a few months.
• Deliverable D3.3 “Report on demonstration of anisotropic TADF emission in thin films” was submitted on schedule.

WP4 Emitter Layer Design and White Stack Integration
• Novaled has tested a number of potential reference TADF emitters in OLEDs.
• Novaled optimised OLED architectures (PIN) on commercially available materials using the first batch of ICT-emitters synthesized by TUD.
• Novaled has further developed the charge transport layers of blue PIN OLED stacks.
• Novaled has tested and optimized a new blue TADF emitter referred to as “Superblue” provided by UDUR.
• Deliverable D4.1 “Design report on optimised blue PIN OLED stacks using TADF materials” was submitted on schedule.

WP5 OLED Lighting Panel Demonstrators
• Astron-FIAMM conducted an evaporation analysis on the candidate electron transporting layer materia
Progress beyond the state of the art and expected potential impact (including the socio-economic impact and the wider societal implications of the project so far)

"Progress beyond the state of the art
The consortium has published 17 research papers in international refereed journals. This includes a paper by Durham University researchers entitled “Revealing the spin-vibronic coupling mechanism of thermally activated delayed fluorescence” published in Nature Communications.

TU Dresden has filed three patents based on their research in the project:
• Patent 1: “”Blaue Fluoreszenzmitter“”, no 10 2015 101 767.9. This TADF material “Blue 1” offers weaker acceptors providing larger charge transfer gaps.
• Patent 2: “”Neue Emittermaterialien und Matrixmaterialien für optoelektronische und elektronische Bauteile, insbesondere OLED“”, no 102015 122 869.6. This TADF material “Blue 2” offers D-A-D and A-D-A molecules with high transitions of D and of A.
• Patent 3: “”Effiziente lichtemittierende Emittermoleküle für optoelektronische Anwendungen durch gezielte Verstärkung der Emission aus ladungsseparierten CT-Zuständen auf Basis dual fluoreszierender Benzol-(Poly)carboxylat-Akzeptoren“”, no 10 2016 110 970.3. These “Blue 3” TADF materials show large dihedral angles between donor and acceptor groups.

Expected potential impacts
The PHEBE project will help to create the expected impacts of call ICT 29 – 2014 Development of Novel Materials and Systems for OLED lighting."

Related information

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