Poster

Structure elucidation of two different materials with TADF properties using three-dimensional electron diffraction

Melanie Bauer, Ute Kolb, Robert Graf, Constantin Haese

Centre for High Resolution Electron Microscopy (EMC-M), Johannes Gutenberg-University Mainz

mbauer07@students.uni-mainz.de, kolb@uni-mainz.de

In the world of modern electronics and lighting technology, optical light-emitting diodes (LEDs) are a major innovation, offering energy-efficient, versatile and environmentally friendly solutions for various applications [1]. Among them, Thermally Activated Delayed Fluorescent (TADF) diodes stand out for overcoming limitations of conventional phosphorescent organic LEDs (OLEDs), particularly regarding their dependence on expensive rare earth metals and their limited operating life. TADF materials utilize the principle of Reverse Intersystem Crossing (RISC) to achieve highly efficient light emission by converting triplet excitons into singlet excitons, enabling the efficient use of singlet and triplet excitons for fluorescence. The unique mechanism of TADF offers several key advantages over conventional OLED technologies. Firstly, TADF materials exhibit exceptionally high internal quantum efficiency (IQE), approaching 100%, which translates to brighter and more energy-efficient devices. Secondly, TADF enables the utilization of abundant and sustainable organic molecules as emitters, paving the way for cost-effective and environmentally friendly LED technologies [2].

In the field of TADF emission diodes, the choice of emitter materials plays a decisive role in the performance and efficiency of the devices. Ideal emitter materials for TADF applications have specific molecular properties that facilitate efficient reverse intersystem crossing (RISC) processes, enabling the conversion of triplet excitons into singlet excitons [2]. The choice of emitter material is critical to TADF performance, with donor-acceptor (D-A) systems being the preferred choice. The spatial separation of electron-rich and electron-poor regions within D-A molecules promotes efficient charge transfer excitations and facilitates the formation of singlet and triplet excitons required for TADF. Common donor groups include aromatic groups such as triarylamine or carbazole, while acceptor groups include cyano, dicyanovinyl or diketopyrrolopyrrole groups [3]. Understanding the solid-state organization of materials is key to minimizing sensitivity to carrier traps and optimizing device performance.

In the following study, we present the structure elucidation of two different materials with TADF properties, using three-dimensional electron diffraction (3DED). Equivalent acceptor units, including a triazine ring with para-fluorinated phenyl rings attached at two positions, characterize these molecules. The third carbon position on the triazine heterocycle is linked to a central phenyl ring attached to a variable amount of unsubstituted carbazole donors, two carbazole donors (OS20) and three carbazole donors (OS30). The crystal structure of the material OS20 could be solved in the space group Pna21 with the oP cell parameters a=29.84 Å; b=28.93 Å; c=4.08 Å. Each unit cell contains four OS20 molecules, which are twisted against each other in such a way that the carbazole residues of one molecule face the outer phenyl groups of the other molecule. Due to the steric hindrance, the carbazole units are arranged at an angle of about 130° to the connecting phenyl ring. For this reason, the molecules do not lie flat in the unit cell but are tilted towards each other. The carbazole units and the phenyl residues are stacked on top of each other in the c-direction, which enables a π-π interaction of the aromatic systems. The distance between the molecular planes is 4 Å.

The material OS30 contains several crystalline phases as presumably also the material OS20, in which 3 different structures, one secondary phase and two different OS30 structures could be identified and solved. The secondary phase is a phenyl ring substituted with four carbazole donor units. The structure was found in the space group C2/c with the mC cell parameters a=31.64 Å; b=10.06 Å; c=25.79 Å; β=103,8°. Both OS30 structures could be solved in space group P-1. The cell parameters of the smaller unit cell are a=9.47 Å; b=13.17 Å; c=18.19 Å; α=98.8°; β=92,2°; γ=98.3° while those of the larger cell are a=8.98 Å; b=29.20 Å; c=33.88 Å; α=97.4°; β=96.8°; γ=93.6°.

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