Electroluminescent Materials for Light-Emitting Electrochemical Cells

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Electroluminescence is an optical phenomenon in which electrical energy is transformed into luminous energy. Light-emitting electrochemical cells (LECs) are a new type of electroluminescent devices that incorporate a thin film (< 100 nm) of an ionic material, usually an ionic transition-metal complex (iTMC), as the electroactive component (Figure 1). Since the iTMC material simultaneously satisfies the requirements of electron and hole injection, charge transport, and luminescence, LECs are much simpler devices than organic light-emitting diodes (OLEDs). Additionally, due to their operation mechanism, air-stable electrodes can be used in LECs which allows a non-rigorous encapsulation of the device. The industrial implementation of LECs for lighting applications is, however, limited by their short lifetimes and color gamut.

The major breakthroughs concerning color, efficiency, turn-on time, and stability in iTMC-based LECs have been achieved using heteroleptic Ir(III) complexes (Ir-iTMCs), which incorporate two negatively charged cyclometalated C^N ligands and one neutral N^N ancillary ligand. The performance of the device has been improved by appropriate tuning of the photophysical and electrochemical properties of the iTMCs through the attachment of peripheral substituents that modulate the HOMO/LUMO energies and modify the nature and emission energies of the excited triplet states.[1,2] Theoretical calculations are especially useful in investigating the relative energy and the electronic nature of the excited states that determine the photophysical properties of iTMCs. They are also very helpful in systematizing the effect that different ligands and substituents have on those properties.

In this presentation we discuss the electronic structure and photophysical properties of a series of heteroleptic Ir-iTMCs used in LECs on the basis of DFT/TD-DFT calculations and we analyze their implications in the device performance. Theoretical calculations have been very helpful in defining a strategy that has lead to highly efficient LEC devices with stability values of thousands of hours by using supramolecularly-caged Ir-iTMCs as the single active component.[3] The tuning of the emission color and, in particular, the design of efficient blue emitters is a main target for the development of white-light emitting devices.[4,5]

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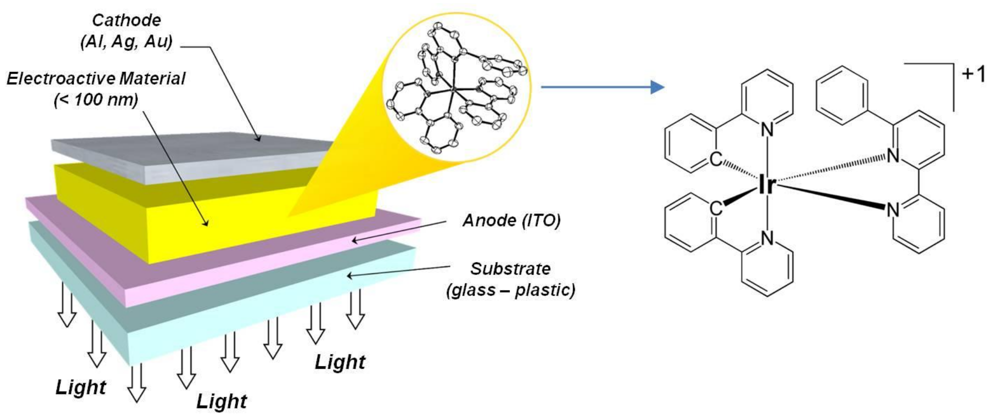

Figure 1. Schematic representation of the simple architecture of a light-emitting electrochemical cell (LEC) device using the $[Ir(ppy)_2(pbpy)][PF6]$ complex as the single active component.