Film morphology of acrylonitrile materials deposited by a solution process and vacuum evaporation. Supramolecular interactions, optoelectronic properties and an approximation by computational calculations.
Film morphology of acrylonitrile materials deposited by a solution process and vacuum evaporation. Supramolecular interactions, optoelectronic properties and an approximation by computational calculations†

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Unsaturated acrylonitrile compounds with a pyridine scaffold are fluorescent materials with efficient solid-state emission and electroluminescence properties. In this work, three low molecular weight compounds, i.e., small molecules, with the donor group 4-(diphenylamino)phenyl (D) and a pyridine-substituent as an acceptor (A) attached to α,β-unsaturated nitrile and one with phenyl were used as the emissive layer in OLEDs. The emissive layer was deposited by either a solution or high vacuum evaporation process to provide insight into the effect of morphology differences on the OLED performance. Notably, for the solution process the better morphology was achieved with dioxane. For devices two cathodes were used, evaporated aluminum and the eutectic alloy Field’s metal composed of Bi, In and Sn, which was deposited by drop casting. Independent of the used cathode and the technique for its deposition, the device performance for both cathodes was similar. Electrical properties such as the threshold voltage, about 3–8 volts, and the current density were affected by the chemical structure of the emitting material, but not by the metal used as a cathode. Results showed that the eutectic alloy is a good alternative as a cathode in organic light emitting diodes. Also, we reported the quantitative analysis of intermolecular interactions by PIXEL and density functional theory (DFT) calculations.

Introduction

Organic light-emitting diodes (OLEDs) have attracted considerable attention due to their potential real-world applications in flat-panel displays and solid-state lighting.1–8 In recent years, numerous organic electroluminescent (EL) materials including polymers and small organic molecules have been thoroughly studied for their application in OLEDs. However, some problems in device manufacturing remain a challenge because the OLED performance depends on the preparation conditions, such as the nature of the emitting compound, the fluorescence quantum yield, a solution or vacuum deposition process, film thickness control, etc. Regarding film deposition there are two common approaches involved: (i) for devices based on small molecules, the standard fabrication method is vapor deposition under a high vacuum and (ii) for polymeric based devices, a simple solution process such as spin-coating or ink-jet printing can be used.2,4 Small molecules have advantages in terms of easy synthesis and purification and vapor deposition techniques allow fabrication of complicated multiple layer structures with excellent device performance.9–13 However, fabrication of such devices by thermal evaporation also increases the complexity and makes the use of small molecules in OLEDs very low.14 Additionally, pixelation using evaporation masks would limit the scalability and resolution.15 The best way to improve the efficiency of fabrication and reduce the production cost of OLEDs is the use of solution processes. For example, ink-jet printing can be effectively used to fabricate large-area, high-resolution full-color flat-panel displays.16,17