

The role of local environment on the electronic properties of a novel blue-emitting donor-acceptor compound

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With the rising popularity of organic light-emitting diodes (OLEDs) in display applications, demand for more efficient blue emitters has increased. We have recently synthesized a novel blue-emitting, donor-acceptor system employing carbazole as the donor and a benzothiazole derivative as the acceptor, BTZ-CBZ. We find that the solution-phase emission of BTZ-CBZ is highly dependent on solvent dielectric, both in lineshape and emission maximum, showing a Stokes shift of 50 nm in methylcyclohexane and 150 nm in acetonitrile. This is expected behavior for donor-acceptor compounds due to the presence of a charge-transfer excited state. However, this large solvatochromic shift is significantly suppressed when BTZ-CBZ is confined to a rigid matrix. Low-temperature emission measurements of BTZ-CBZ in frozen solvent glass matrices show Stokes shifts closer to 80 nm, exhibiting little variation with glass polarity. In addition, BTZ-CBZ cast in soft polymer matrices of differing polarities showed similar behavior. We theorize that solvent reorganization plays a significant role in the relaxation mechanism of the BTZ-CBZ excited state. In this work, we describe our use of different spectroscopies and electronic structure calculations to probe the nature of the Franck-Condon and emissive states. The behavior of BTZ-CBZ in rigid matrices has direct implications on its viability as a blue emitter in solid-state OLEDs.