Examining Ambipolar, Nitrogen-Doped Polycyclic Aromatic Hydrocarbons for Enhanced Efficiency in TADF OLED Emission

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Recently, researchers have shown increasing interest in thermally activated delayed fluorescence (TADF) materials, especially for their potential in advancing organic light-emitting diodes (OLEDs) [1]. These materials utilise electrically generated triplet excitons, converting them into emissive singlet excitons through reverse intersystem crossing (rISC) and receiving IQE of up to 100%. Our investigation explores how the electron-donating capabilities of a novel class of emitters, nitrogen-doped polycyclic aromatic hydrocarbons (PAHs), affect their photophysical properties. These molecules aim to narrow the gap between the highest occupied (HOMO) and lowest unoccupied molecular (LUMO) orbitals, resulting in minimal singlet-triplet gaps (ΔE_{ST}), crucial for efficient rISC operations [2]. All compounds examined displayed small ΔE_{ST} values ranging from 0.03 to 0.37 eV, indicating favourable TADF properties. To characterise these nitrogen-doped PAHs, we conducted comprehensive analyses, including electrochemistry, photophysical, and device fabrication. By modifying the molecular structure with various electron-donating groups, we could control the luminescence mechanism, shifting between TADF and room-temperature phosphorescence (RTP) and enhancing photoluminescence quantum yields (PLQY) up to 96% in solid thin film matrices such as Zeonex® and CBP. Time-resolved spectroscopy performed on these matrices revealed detailed emission properties of the compounds. To demonstrate feasibility, we constructed solid-state OLED devices using CBP as the host material. We achieved a turn-on voltage of around 4.0 V and reached a maximum external quantum efficiency (EQE) of up to 21.9% by incorporating phenothiazine as the donor component.

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