TRI/TETRAPHENYLETHENYLCOUPLED PHENOXAZINE AND PHENOTHIAZINE BASED HIGHLY FLUORESCENT MATERIALS SHOWINGAIEE FOR OLEDS

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In order to develop effective blue emitters for organic light-emitting diodes (OLEDs), this work intends to synthesise three compounds based on phenoxazine and phenothiazine that are coupled with phenylethenyl using a single-step Buchwald-Hartwig approach. Results from photophysical studies suggest that, with increasing water percentage, compound dispersions in water-THF mixes exhibit strong aggregation-induced enhanced emission (AIEE). Cyan fluorescence is the most intense emission. Toluene solutions of the compounds have photoluminescence quantum yields ranging from 3-26%, and solid films have values ranging from 13.5-53%. The AIEE phenomenon is thought to be responsible for this finding. Computational simulations grounded on density functional theory were used to quantify intramolecular charge transfer, dihedral angles, border molecular orbitals, excitation energies, and wavelengths. Analyses of compounds' internal reorganisation energies, grounded on Marcus theory, reveal high levels of hole mobility. Cyclic voltammetry estimates the ionisation potentials and electron affinities of the compounds to be between 5.15 and 3.31 eV and 2.08 and 2.24 eV, correspondingly. Blue-cyan emission with an electroluminescence maximum of around 500 nm is shown by OLEDs built employing synthetic compounds as the host. External quantum efficiencies of 2.5–6% and brightness levels exceeding 1000 cd/m^2 are characteristics of the manufactured devices.