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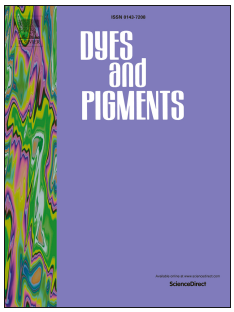

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Synthesis and photophysical properties of new perylene bisimide derivatives for application as emitting materials in OLEDs

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Abstract

Three novel perylene diimide derivatives with bulky aromatic moieties (fluorene, carbazolyl-fluorene, and anthracyl-fluorene) connected via triple bonds with perylene core were successfully designed and synthesized. The chemical structure of prepared compounds was confirmed by ^{1}H and ^{13}C NMR and mass spectrometry. Their optimized ground-state geometry and frontier molecular orbitals were theoretically estimated based on density functional theory. The compounds undergo the reversible electrochemical reduction process and exhibit very low energy band gaps (1.56-1.98 eV) being promising for electronic applications. They also display excellent solubility, high thermal stability and luminescence in solution and in the solid state as a film in the red spectral region. The highest photoluminescence quantum yield (79 % in solution and 28 % in the film) was found for perylene diimide bearing fluorene unit. All molecules showed the ability for light emission under an applied voltage. The fabricated diodes with structure ITO/PEDOT:PSS/compound/Al exhibited electroluminescence with maximum emission band located between 685 and 732 nm. The most intense electroluminescence, which was additionally plasmonically enhanced by incorporating silver nanowires, was observed for the device based on molecules with anthracene structure.