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Synthesis and characterization of new conjugated azomethines end-capped with amino-thiophene-3,4-dicarboxylic acid diethyl ester

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A new series of thiophene-based azomethines differing in the core structure was synthesized. The effect of the central core structure in azomethines on the thermal, optical and electrochemical properties was investigated. The obtained compounds exhibited the ability to form a stable amorphous phase with a high glass transition temperature above 100 °C. They were electrochemically active and undergo oxidation and reduction processes. The highest occupied (HOMO) and the lowest unoccupied molecular (LUMO) orbitals were in the range of −3.86–−3.60 eV and −5.46–−5.17 eV, respectively, resulting in a very low energy band gap below 1.7 eV. Optical investigations were performed in the solvents with various polarity and in the solid state as a thin film deposited on a glass substrate. The synthesized imines absorbed radiation from 350 to 600 nm, depending on its structure and showed weak emission with a photoluminescence quantum yield below 2.5%. The photophysical investigations were supported by theoretical calculations using the density functional theory. The synthesized imines doped with lithium bis-(trifluoromethanesulfonyl)imide were examined as hole transporting materials (HTM) in hybrid inorganic-organic perovskite solar cells. It was found that both a volume of lithium salt and core imine structure significantly impact device performance. The best power conversion efficiency (PCE), being about 35–63% higher compared to other devices, exhibited cells based on the imine containing a core tiphenylamine unit

Metryczka

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