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THEORETICAL APPROACH TO OLED AND OTFT MATERIALS: MOLECULAR DESIGN AND CHARACTERIZATION

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During the last decade, organic pi-conjugated materials have become one of the most interesting topics in the applications of optoelectronic and electronic devices such as organic light-emitting diodes (OLED) and organic thin-film transistors (OTFT). The performance of these devices depends highly on the alignment of frontier molecular orbital energy levels and efficiency of the charge-transport processesof organic layers in these devices. Here, quantum-mechanical methods are applied in order to characterize the nature of electronic structures and hopping processes in hole and electron transport materials used in OLED and OTFT devices. Calculatedionization potentials and optical gaps are well compared with available experimental data. Intramolecular reorganization energies are also estimated to help understanding of hole- and electron-vibrational couplings in OLED and OTFT materials. Thus, the results obtained by theoretical calculations can be guidelines for the rational design of new materials for OLED and OTFT.