Special Issue

Design and Synthesis of Organic Materials for OLED Applications

Message from the Guest Editor

As OLEDs gain widespread commercial use, the demand for improved emissive materials, especially those delivering efficient and stable blue, red, and green emission, continues to grow. Research progress in phosphorescent and thermally activated delayed fluorescence (TADF) materials has helped address performance gaps. Density functional theory (DFT) calculations play a crucial role in guiding molecular design, enabling the prediction and optimization of key electronic and optical properties prior to synthesis. This Special Issue presents a comprehensive review of recent advances in both organic emissive materials and device-engineering approaches. It maps out the landscape of materials under exploration, including small molecules, conjugated polymers, organometallic complexes, perovskite-based systems, and carbon dots. In addition, the review highlights progress in multilayer OLED device architectures, focusing on organic interfacial layers such as PEDOT:PSS alternatives, charge injection/transport layers, and cathode/anode modifiers.

Guest Editor

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Deadline for manuscript submissions

closed (31 March 2026)

Molecules

an Open Access Journal by MDPI

Impact Factor 4.6
CiteScore 8.6
Indexed in PubMed

mdpi.com/si/250187

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As the premier open access journal dedicated to molecular chemistry, now in its 30th year of publication, the papers published in *Molecules* span from classical synthetic methodology to natural product isolation and characterization, as well as physicochemical studies and the applications of these molecules as pharmaceuticals, catalysts, and novel materials. Pushing the boundaries of the discipline, we invite papers on all major fields of molecular chemistry and multidisciplinary topics bridging chemistry with biology, physics, and materials science, as well as timely reviews and topical issues on cutting-edge fields in all of these areas.

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