

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

Dr. Dalius Gudeika

Institute of Data Science and Digital Technologies, Vilnius University,
Akademijos Str. 4, 08412 Vilnius, Lithuania

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Molecules
Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland
Tel: +41 61 683 77 34
molecules@mdpi.com

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Message from the Editor-in-Chief

As the premier open access journal dedicated to molecular chemistry, now in its 29th 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.

Editor-in-Chief

Prof. Dr. Thomas J. Schmidt

Institute of Pharmaceutical Biology and Phytochemistry, University of Münster, Corrensstrasse 48, D-48149 Münster, Germany

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