Communications in Computational Chemistry
Commun. Comput. Chem., Vol. 7, No. 3, 181–189
doi: 10.4208/cicc.2025.126.02
Regular Article

Recent Progress of Machine Learning on Organic Optoelectronic Materials

Jinglei Fu[1], Shichen Zhang[1] and Xiaoyan Zheng[1, *]

[1]Key Laboratory of Cluster Science of Ministry of Education, Key Laboratory of Medicinal Molecule Science and Pharmaceutics Engineering of Ministry of Industry and Information Technology, Beijing Key Laboratory of Photoelectronic/ Electro-photonic Conversion Materials, School of Chemistry and Chemical Engineering, Beijing Institute of Technology, Beijing 100081, P. R. China.

[*] Corresponding authors: xiaoyanzheng@bit.edu.cn (Xiaoyan Zheng)

Received on 6 May 2025; Accepted on 2 June 2025

Abstract: Organic optoelectronic materials, owing to their exceptional photoelectronic properties, have extensive applications across diverse fields, such as lighting and display, photovoltaic devices, and bioimaging. Machine learning (ML) provides new opportunities for advancing research on organic optoelectronic materials. ML leverages existing datasets to establish robust input-output correlations for predicting material properties, thereby substantially reducing computational costs and enhancing efficiency. This review comprehensively explores recent progress on ML applications for organic optoelectronic material. We focused on three key aspects. First, we review applications ML in predicting photophysical properties of organic dyes, including absorption/emission wavelengths, quantum yields, and aggregation-induced emission/aggregation-caused quenching effects. Second, we examine ML applications in predicting subcellular targeting of fluorescent probes. Third, we discuss the role of ML in screening key descriptors for organic photovoltaics material. The advances in data science position ML as a pivotal tool for elucidating intricate structure-property correlations in molecular systems, driving the accelerated innovation of optoelectronic devices.

Key words: machine learning, organic luminescent materials, OPV materials, fluorescent probes.

1. Introduction

Organic optoelectronic materials have emerged as pivotal components in organic light emitting diodes (OLEDs)[1-3], fluorescent probes [2,4-5], and organic solar cells (OSCs)[6]. These materials have been used across diverse environments, including dilute solution, thin films, and crystalline states, where critical performance metrics, such as luminescent color, quantum efficiency, and lifetime, are highly sensitive to subtle change of environments [7-9]. Minor change of chemical structures of organic optoelectronic molecules significantly alters their macroscopic properties, which brings huge challenges in the rational design and performance optimization of organic optoelectronic materials.

Currently, the development of organic optoelectronic materials has largely based on experimental trial-and-error approaches, which are time-consuming and high-cost. Alternatively, theoretical calculation is an effective way to complement experimental techniques in molecular design of organic optoelectronic materials. Mul tiscale modeling approaches, including quantum mechanism (QM) [10-13], quantum mechanics/molecular mechanics (QM/