

Abstract

Rate of Radiative and Non-Radiative Processes in Electro-Optical Devices: a Theoretical Study

Organic materials for optoelectronic applications are at the forefront of current scientific research, offering promising alternatives to traditional inorganic semiconductors. Because of their eco-friendliness, ease of fabrication, and broad chemical tunability make them attractive candidates; however, challenges such as limited stability, low efficiencies, and environmental sensitivity continue to limit their performance. Addressing these challenges requires a detailed understanding of the relationships between molecular structure, optoelectronic properties, and device performance.

Theoretical approaches provide a powerful route to this understanding by enabling the rational design of molecules and polymers prior to synthesis. In this thesis, a novel and accurate theoretical approach for treating internal conversion is introduced, combining computational tractability with physical rigor. This model allows quantitative predictions of the rate constants of elementary radiative and non-radiative electronic transitions which take place in modern optoelectronic devices, allowing for analysing competitive de-excitation pathways, which could affect device efficiencies.

The predictive capability of this approach facilitates the design of materials with tailored photophysical and electronic properties. This is particularly relevant for next-generation optoelectronic devices, including OLEDs with improved quantum yields, organic solar cells with minimized recombination losses, and flexible or large-area molecular electronics. By linking theoretical insights directly to material optimization, this work provides a framework for the accelerated discovery and development of organic materials that combine efficiency, stability, and tunability in advanced optoelectronic technologies.