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Decoding Photoluminescence Origins in Carbon Dots: A Molecular Fluorophore Perspective

Understanding the origin of photoluminescence (PL) in carbon dots (CDs) remains a fundamental challenge due to the structural diversity and chemical complexity arising during their synthesis. While early hypotheses attributed PL primarily to carbogenic cores, mounting evidence points to molecular fluorophores (MFs) and their dynamic interactions within the CD matrix as key contributors to the observed emission.[1, 2] In this contribution, we present a computational investigation into the nature of emissive states in CDs, focusing on the role of embedded or surface-bound fluorophores and their communication with surrounding domains.[3] Using density functional theory (DFT) and time-dependent DFT, we explore how noncovalent interactions, covalent bonding, and π–π stacking between MFs and functionalized polyaromatic fragments modulate excited-state properties.[4] These studies reveal the formation of charge-separated states and the conditions that promote energy or electron transfer between emissive domains. Furthermore, complementary molecular dynamics (MD) simulations of oligomer aggregation provide insight into the organization of less-ordered CD-like environments and the localization of their emissive sites. By integrating electronic structure calculations with structural models derived from MD, we elucidate how fluorophore arrangement and local electronic environments govern emission wavelength, and deactivation pathways. This multi-scale framework enhances our mechanistic understanding of PL in CDs and paves the way for rational design of materials with tailored emission characteristics.

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