TRIGGERING EXCITED STATE DYNAMICS IN GRAPHENE QUANTUM DOTS: THE ABSORPTION SPECTRUM OF CORONENE AND CIRCUMCORONENE

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Graphene quantum dots (GQD) are nanoparticles consisting of a single or several layers of graphene sheets whose thickness does not exceed 100 nanometers. GQD have become extremely popular in optoelectronics as nanocarriers for cancer therapy drugs and in bioimaging techniques, mostly due to their ease of preparation, biocompatibility and tunable absorption and emission properties.[1]

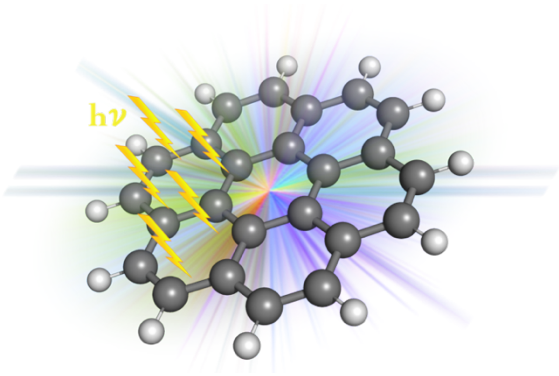

Figure 1: Visualization of the fluorescence and phosphorescence emission of coronene via excited state deactivation.

This work is focused on coronene (Fig. 1), the smallest unit of a graphene nanoflake and zero-dimensional quantum dot. Several studies have found that coronene shows fluorescence and phosphorescence in the visible range of the light spectrum.[2] As a starting point, the excited state deactivation pathways of a single unit of coronene are unravel using the ML-MCTDH method [3] and a vibronic coupling model for the nuclear Hamiltonian, including both singlet and triplet states. This study has been extended to circumcoronene in the direction towards graphene where promising results has been found.

Future work will look at expanding the system size, adding further layers, and pondering the effect of functionalization to explain the strong emission found by our experimental collaborators in doped carbon nanoparticles.[4]

References

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