

Study of C₆₀ fullerene photoinduced functionalization for room temperature single photon generation

B. Berasategui Migueliz^{1,3,*}

R. Lahoz Sanz^{2,3}

C. Becerra Gómez³

S. Hernández Márquez¹

J. M. Gómez Cama^{1,3,4}

B. Juliá Díaz^{2,3}

¹ Departament d'Enginyeria Electrònica i Biomèdica, Universitat de Barcelona (UB)

² Departament de Física Quàntica i Astrofísica, Universitat de Barcelona (UB)

³ Institut de Ciències del Cosmos (ICCUB), Universitat de Barcelona (UB)

⁴ Institut d'Estudis Espacials de Catalunya (IEEC)

*benat.berasategui@ub.edu

C₆₀ fullerene embedded in polystyrene exhibits on-demand single-photon emission at room temperature, making it a promising candidate for scalable quantum communication devices [1]. However, pristine C₆₀'s icosahedral symmetry suppresses the lowest-energy HOMO-LUMO transition, predicting negligible photoluminescence. It has been hypothesized that photo-oxidative functionalization, forming C₆₀O_n species, breaks the molecular symmetry and activates previously forbidden transitions [2]. To test this idea, we study thin films of C₆₀ embedded in a polystyrene matrix under continuous 405 nm excitation, to monitor spectral evolution.

Upon irradiation, the photoluminescence spectrum undergoes measurable changes (Figs. 1 and 2) before reaching saturation, consistent with progressive functionalization of individual C₆₀ molecules. Control experiments show that neither pure polystyrene nor pristine C₆₀ films exhibit similar spectral changes under identical conditions. These observations support the inference that photo-oxidative functionalization requires both C₆₀ and the polymer matrix and is responsible for the observed emission. Identifying the dominant

C₆₀O_n species and clarifying the detailed functionalization mechanism will guide the design of future C₆₀-based quantum light sources.

References

- [1] R. Lahoz et al, Nano Letters 25, (2025) 15048-15054.
- [2] C. Zhang et al, Physics Letters 68, (1996) 943-945.

Figures

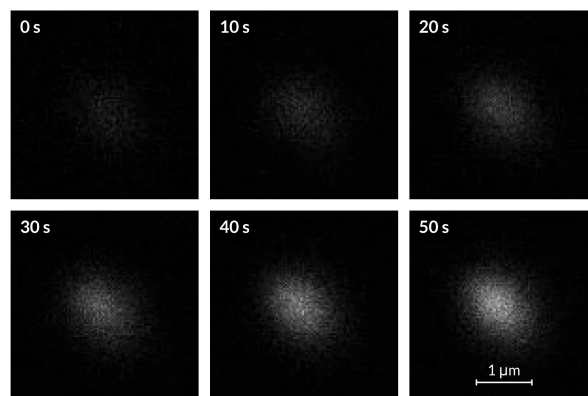


Figure 1: Micrographs showing the photoluminescence intensity increase when a thin film of C₆₀ embedded in a polystyrene matrix is continuously irradiated with a 405 nm laser.

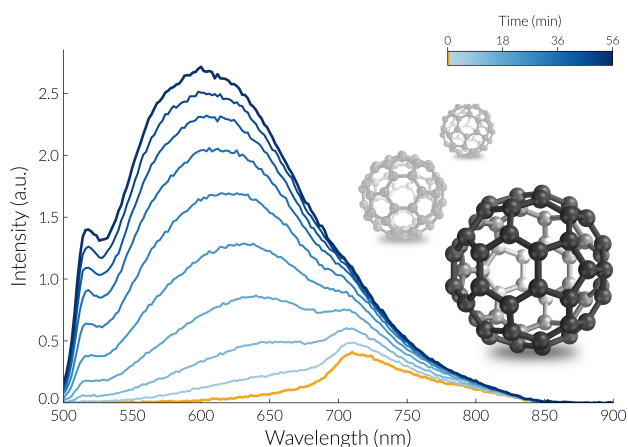


Figure 2: The photoluminescence spectrum of the sample shifts from approximately 710 nm to 600 nm and the intensity increases by a factor of four. The yellow trace corresponds to the spectrum of pristine C₆₀.