Diameter-dependent single- and double-file stacking of squarylium dyes inside single-wall carbon nanotubes

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The filling of single-wall carbon nanotubes (SWCNTs) with dyes has become a novel path to add and create new functionalities through the mutual interaction between the confined dyes and host SWCNTs. In particular cases, the encapsulated dyes form strongly interacting molecular arrays that result in severely altered optical properties of the dyes^{1–3}. In this work we report for the first time the combination of extensive chirality-sorting⁴ and dye filling, leading to the isolation of nearly single chirality squarylium-filled SWCNTs as shown in the photoluminescence-excitation (PLE) map presented in Figure 1.

For each dye@SWCNT chirality combination we observe a different absorption wavelength of the confined dyes, originating from the different dye stacking driven by the diameter of the surrounding SWCNT. This diameter-dependent dye absorption is experimentally determined through the measurement and detailed fitting of fluorescence-excitation maps of different chirality-sorted dye-filled SWCNT samples, where for each dye@SWCNT combination a different energy transfer peak is observed.

We therefore demonstrate that the diameter of the SWCNT is a lever to tune optical properties of the hybrids, paving the way for future applications in optoelectronics. Moreover, comparison with molecular models provides access to the possible different stacking configurations of the dyes inside the hollow space of SWCNTs with different diameters.



Figure 1 Example of a PLE map and the corresponding fit for one of the 15 samples: (a) Experimental PLE maps; The white dots represent all the chiralities that have been fitted and the crosses represent the energy transfer peaks. (b) Fitted PLE map, the most abundant chirality is labelled.

References

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