

# Diameter-dependent stacking of dye molecules inside single-wall carbon nanotubes

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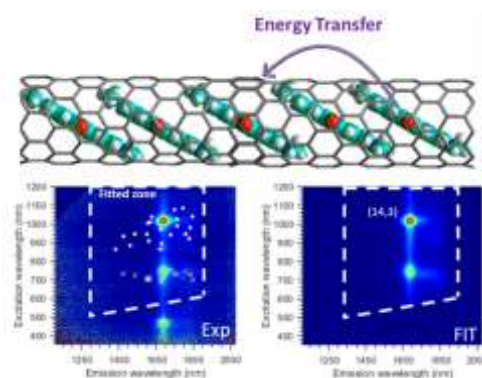
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Thanks to the extensive variability of chiral structures of SWCNT, a large variety of electronic and optical properties can be accessed, making them extremely promising for diverse applications such as solar energy harvesting and high-performance (opto-)electronic devices. Besides these very peculiar intrinsic properties, SWCNTs also exhibit a hollow core, which can be filled with dyes giving rise to new one-dimensional hybrids that merge the properties of the nanotube with those of the dyes<sup>1-2</sup>. In this work<sup>3</sup> we report for the first time the combination of extensive chirality-sorting<sup>4</sup> and dye filling, leading to the isolation of nearly single chirality squaraine-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 followed by an energy transfer, is experimentally determined through the measurement and detailed fitting of fluorescence-excitation maps of different chirality-sorted dye-filled SWCNT samples. 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.

## References

- [1] S. Cambré et al., *Nature Nanotechnology* 2015, 10 (3), 248–252.
- [2] S. Van Bezouw et al., *ACS Nano* 2018, 12 (7), 6881–6894
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## Figures



**Figure 1:** (top) Schematic view of the new hybrids (bottom) Example of a PLE map and the corresponding fit for one of the 15 samples. (left) experimental PLE maps, the white dots represent all the chiralities that have been fitted and the crosses represent the energy transfer. (right) Fitted PLE map, the most abundant chirality is labelled.