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Nonperturbing, conjugation-preserving covalent functionalization of single-walled carbon nanotubes

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The most common outcome of covalent treatments of carbon nanotubes is the conversion of sp2 carbon atoms into their sp3 hybridization state. Even mild approaches interrupt the conjugation of the carbon network with detrimental effects on their optoelectronic properties. Cycloaddition reactions establish covalent bonds through pi-electrons to bridge targeted functionalities onto the tubes. The carbon atoms below the bridge are converted into the sp3 state (closed configuration, Fig. 1a) or, if the C-C bond below the bridge is released, keep their sp2 character (open configuration, Fig. 1b) and preserve the overall conjugation of the extended network. We have recently demonstrated that the outcome of a triazine-based [2+1] cycloaddition reaction results in the open configuration (Fig. 1c) and preserves the intrinsic properties of the tubes, even at high degrees of functionalization (4%) [1]. Here we will highlight some of the benefits of this approach, such as the preservation of their radiative emission (Fig. 1d) or the fine-tuning of the position of their Fermi levels.
We will moreover discuss how the functionalized tubes can be exploited as starting platform for advanced materials. We show how the attachment of molecular systems makes them integrating part and in electronic communication with the conjugated network of the tubes, yielding new ways to non-perturbatively tailor, control, and alter the optical response of the tubes for novel applications. The conjugation of the molecular switch spyropiran-merocyanine, for example, enables controlled on-off switching of the tubes'emission to be exploited for nanotubes-based super-resolution microscopy.

[1] A. Setaro, *et al.*, Nat. Comm. **8**, 14281 (2017).

Summary

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