Diameter-dependent optical absorption and energy transfer from encapsulated dye molecules to single wall carbon nanotubes

Sofie Cambré[1], Stein van Bezouw[1], Dylan H. Arias[2], Rachelle Ihly[2], Andrew J. Ferguson[2], Jochen Campo[1], Justin C. Johnson[2], Joeri Defillet[1], Wim Wenseleers[1] and Jeffrey L. Blackburn[2]

[1] *Physics Department, University of Antwerp, Universiteitsplein 1, B-2610 Antwerp, Belgium*
[2] *Chemistry & Nanoscience Center, National Renewable Energy Laboratory, Golden, Colorado 80401, United States*

The hollow core and well-defined diameters of single-walled carbon nanotubes (SWCNTs) allow for creation of unique one-dimensional hybrid structures by encapsulation of various molecules. For instance, we previously demonstrated that in this way dipolar dye molecules can be naturally aligned in an ideal head-to-tail arrangement to create assemblies with a giant total nonlinear optical response.[1]

Here, we encapsulated specific dye molecules inside the SWCNTs and demonstrate that the optical absorption of the encapsulated dye molecules and subsequent excitation energy transfer (EET) from encapsulated dyes to the SWCNTs is strongly modulated by the SWCNT diameter, implying a diameter-dependent stacking of the molecules inside the SWCNTs. The dye filling and EET are thoroughly characterized by optical absorption, resonant Raman, two-dimensional infrared photoluminescence excitation (PLE) spectroscopy and transient absorption spectroscopy.

In addition, we find that SWCNT filling does not limit the selectivity of subsequent separation protocols (including polyfluorene polymers for isolating only semiconducting SWCNTs and aqueous two-phase separation for enrichment of specific SWCNT-chiralities). The design of these functional hybrid systems, with tunable dye absorption, fast and efficient EET, and possibilities for subsequent separation, demonstrates potential for implementation in photo-conversion devices.

[1] S. Cambré *et al*., Nature Nanotechnol. **10**, 248 (2015)

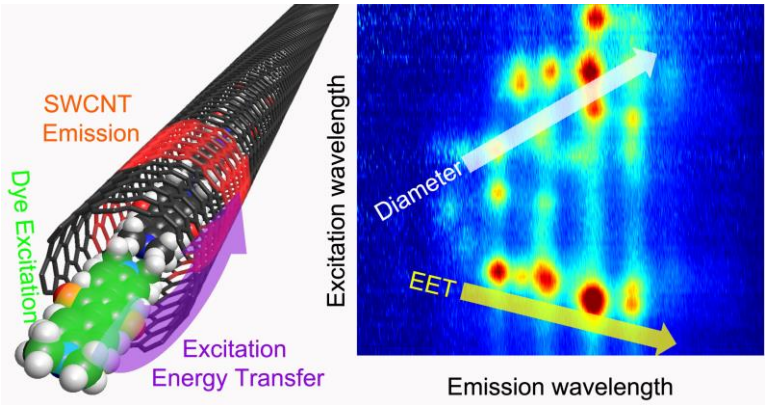

Fig.1 Excitation energy transfer from encapsulated dyes to SWCNTs probed by wavelength-dependent PLE spectroscopy.