

## Charge Transfer in Multifunctional Molecular Materials

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Multifunctional carbon nanostructures are currently under active investigation for producing innovative materials, composites, and optoelectronic devices, whose unique properties originate at the molecular level. Among the wide variety of carbon allotropes recently discovered,  $C_{60}$ , single wall carbon nanotubes (SWNT) and single wall carbon nanohorns (SWNH) are of particular interest.  $C_{60}$  is entirely made of pentagons and hexagons resulting in 0.78 nm sized truncated icosahedral carbon spheres. In contrast, the structure of SWNT has a cylindrical shape, which can be conceptually generated by wrapping a one-atom-thick layer of a graphene sheet into a seamless cylinder. The diameter of most SWNT is around 1 nm – similar to that of  $C_{60}$  – with a tubular length that can reach many thousands of times their diameter. Importantly, based on different arrangements, SWNT possess different electrical properties, which are the result of the electrons moving differently in the tube depending on the SWNT arrangement. SWNH, on the other hand, are typically constituted by tubes of about 2-5 nm of diameter and 30 to 50 nm long, which associate with each other to give rise to round-shaped aggregates of 100 nm of diameter. Their large surface areas and inner nanospaces are of great importance, since they ensure a great affinity, for example, with organic electron donors.

The accomplishment of multiple-performance objectives in a single system necessitates combining these carbon allotropes with other classes of materials. Our past work has mapped out compounds that proved particularly useful: active organic materials such as porphyrins / phthalocyanines and oligomers / polymers. We have demonstrated that linking these molecular building blocks creates enormous synergisms in going much beyond just harnessing the features of the individual subunits or constituents. Eventually it enables the control over molecular arrangement – well-defined ensembles and superstructures with widely differing property values – and results in the development of the necessary tools for fine-tuning properties on the molecular, nanoscale level.

I will highlight the opportunities that rest on fullerenes and single wall carbon nanotubes within the context of charge transfer reactions in novel chemical as well as light driven systems with high tensile strength. A fundamental aspect of our research is to integrate such functions without sacrificing the structural and electronic integrity of the material. In this context, I will survey our concepts to generate functional entities using the bottom up approach, that is, to design, manipulate, characterize, examine, and understand the potential of carbon materials as a novel platform for stable electron donor-acceptor hybrids and conjugates. Important aspects will include the impact, the benefits and some of the promises that evolve from charge transfer reactions involving carbon nanostructures with high tensile strength on i) the stabilization of radical ion pair states, ii) multi electron catalytic reactions, and iii) photoelectrochemical / photovoltaic solar energy conversion.