

# MOLECULAR MATERIALS: CONCEPTION, DESIGN AND APPLICATIONS

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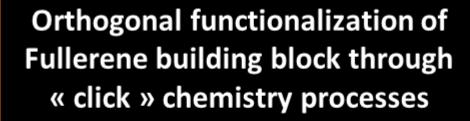
#### List of publications

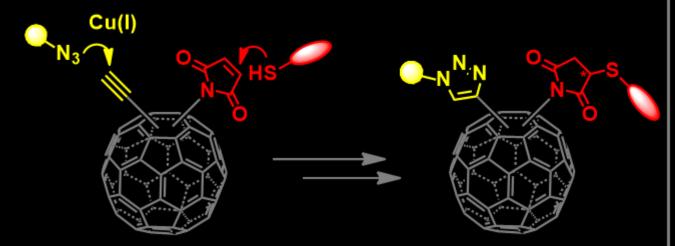
#### **Main themes**

This theme has set out to conceive novel molecular architectures, from their design and synthesis through to their applications. Over the last few years we have concentrated on fullerene chemistry, but also on aromatic molecular structures based on naphthalene, acene, perylene or their derivatives, exploiting the planarity of these pi-conjugated systems, or the spatial deformation of their 3D topologies. These systems have been studied at the molecular level, but also grafted onto surfaces or in the form of thin films.

# **Fullerene C60 chemistry**

This work has allowed the development of a new strategy to functionalise C60 adducts by using two different functional groups with distinct reactivities, which can take part in click chemistry processes (CuAAC reaction and Michael addition). This strategy allowed the design of diversely substituted photo- and electro-active systems. This strategy has also been exploited to associate C60 with helical peptides, with the aim of forming self-assembled mono-layers on gold surfaces, where the peptide helps to structure the mono-layer and aids electron transfer to the metal surface.





Design of new structures for biological and materials sciences

- Photo- and/or electro-active
   Anchorage unit for carbon nanostructures
- Dendronization or cysteine labeling

## **Organic semiconductors**

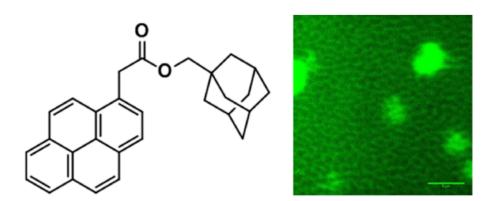
Polycyclic conjugated hydrocarbons are potentially interesting for the construction of optoelectronic devices. Generally, pi-conjugated systems which absorb at over 600nm are poorly stable to the combined action of oxygen and/or light. One of our objectives has been to develop molecules with a small HOMO-LUMO gap to be used as the active layer in field effect transistors. Recently, to achieve this aim, bis-acene type polycyclic hydrocarbon structures or quinoidal structures which incorporate (di)indeno-acene type anti-aromatic sub-units have been synthesized.

(i-Pr)<sub>3</sub>Si 
$$E_g = 1.36 \text{ eV}$$
  $E_g = 1.89-1.71$   $\mu_{\text{hole}} = 1.7 \cdot 10^{-3} \text{ cm}^2 \cdot \text{V}^{-1} \cdot \text{s}^{-1}$   $Si(i-Pr)_3$   $\mu_{\text{hole}} = 0.3 \text{ cm}^2 \cdot \text{V}^{-1}$ 

New fluorescent compounds have been synthesized from diversely functionalised pyrene dibenzoates by using intramolecular Friedel-Crafts reactions and triflic acid as activator. This acid allows control of the reactivity and regioselectivity to obtain the target molecules in excellent yields.

# 2D and 3D Aromatic architectures. Synthesis, modulations and properties

**2D Topology.** The planarity and/or the deformation from a plane of polyaromatic molecules have been exploited to generate structuration effects on surfaces, and control their optical, electronic and wetting properties.



**3D Topology.** Topology control by using helicity parameters and selectively placing substituents or heteroatoms are key points for generating diversity in 3D molecular objects. A theoretical and experimental approach allowed us to show that selective cation (or anion) complexation resulted from the co-operative combination of different weak bonds (Pi-, S- and CO-cation).

