



ΙΤΕ/ΙΕΧΜΗ

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ΘΕΜΑ: Πολυλειτουργικά υλικά νανοδομών άνθρακα.
Multifunctional carbon nanostructures.

ΤΟΠΟΣ: Αίθουσα Σεμιναρίων ΙΤΕ/ΕΙΧΗΜΥΘ

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ΠΕΡΙΛΗΨΗ:

Carbon-based nanostructured materials such as *fullerenes*, *nanotubes* and *graphene* attract the focus of considerable research and scientific interest. This is because each of them can be used as a probe to address the role of dimensionality and confinement in materials at the nanometer scale.

Considering the number of reactive double bonds, controlling the degree of additions to fullerenes is a very challenging task. Nevertheless, sophisticated approaches have been developed in order to chemically control the topological formation of isomers with the most outstanding methodology being the tether-directed remote functionalization. Applying the azomethine ylides cycloaddition functionalization with diformyl-triphenylamine, we succeeded on the selective formation of either the equatorial bisadduct or the dumbbell triad. Our group is also interested on azafullerenes and endohedral metallofullerenes. Azafullerenes derive upon substitution of a carbon atom with nitrogen in fullerene spheres. We have developed a synthetic route that gives access to C₅₉N-based carboxylic acid derivative as key material toward the preparation of diverse



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C₅₉N-based dyads with organic electron donors. On the other hand, encapsulation of metals or metal nitrides within the empty space of fullerenes results on the formation of endohedral metallofullerenes. Electron transfer occurs from the encapsulated metal to the carbon cage while the energy band gap of endohedral metallofullerenes can be varied depending on the fullerene cage, the kind and the number of the encapsulated metal atoms.

Carbon nanotubes (CNTs) as 1D molecular wires possessing delocalized π -electrons, exhibit unusual electronic, mechanical and adsorptive properties, while showing high electron mobility. Polyelectrolytic blocks combined with CNTs assist high dispersion in aqueous media. Moreover, such polyelectrolyte-CNT hybrids act as templates for the *in-situ* formation of monodispersed nanoparticles at the ionic sites generating novel nanostructures. Advantageously, SWCNTs possess fascinating hollow space to accommodate doping materials. A typical example is the so-called peapods, materials in which fullerenes are entrapped inside the empty pseudo-1D nanoscopic space of SWCNTs. Functionalization and solubilization of peapods is a major issue that would allow to study properties in solution – especially when considering the rich electrochemistry of fullerenes – while enable better manipulation and handling, and therefore, practical applications. Moreover, functionalized peapods become more useful than the original ones as the covalently grafted moieties on the outer skeleton of the nanotubes can be tailored for specific applications. On the other hand, carbon nanohorns (CNHs) present features similar to the ones of fullerenes (at sites near the conical-shaped tip) and nanotubes (at sites located away from the conical tip). However, nanohorns are morphologically different from nanotubes as they i) possess a conical-shaped tip, ii) are much shorter in length, and iii) aggregate in spherical superstructures. CNHs can be functionalized by i) covalent attachment of organic units onto their skeleton, and ii) non-covalent supramolecular, van der Waals, π - π stacking interactions and/or coulombic electrostatic interactions with aromatic planar and/or charged organic moieties. Moreover, CNHs accept electrons and more importantly, can readily diffuse them along the cone main axis, with almost negligible loss of energy. Therefore, CNHs can be utilized as electron acceptors towards the formation of hybrid materials with organic electron donors, for application in photovoltaics.

Graphene is an outstanding material, consisting of a two-dimensional (2D) single layer of sp²- hybridized carbon atoms bonded together in a hexagonal “honeycomb” lattice and presents exceptional properties that allow its use in energy conversion and storage systems. In this context, the covalent functionalization of graphene sheets with photoactive molecules such as porphyrin and phthalocyanine has been carried out and most importantly, prototype devices were constructed by fabricating the graphene-based hybrid materials as photoanodes in photoelectrochemical cells, while their efficiency and response were examined.