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Service de Physique de l'Etat Condensé
SÉMINAIRE
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1D Nanostructured Materials. From Catalysis to Molecular Electronics

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In last years, nanostructured forms of bulk materials with a high technological and industrial interest such as delaminated layers, nanoparticles, and nanotubes/wires have focused a wide attention from the Condensed Matter Community. As the dimensionality of an extended bulk material decreases, novel and amazing structural, mechanical and electronic transport properties burgeon at the nanoscale regime. The before-mentioned novel properties, together with a proved easy experimental handling, point out the nanostructured materials as the perfect candidates for their implementation in state-of-the-art catalysis and nano(magneto/opto/electronic) devices, depending on the targeted functionality. In particular, 1D nanostructured materials comprising nanotubes, nanowires, and monoatomic chains nowadays have demostrated to be on the cusp of the wave of the nanostructured materials. In this seminar we will focus on some examples of these 1D materials exhibiting a huge variety of different properties.

As a first example, near the top of any list of candidate catalytic materials are metal oxides, which are already used extensively as (electro/photo-)catalysts. This is partly owing to their high stability in harsh oxidizing environments compared to that of their pure metal counterparts. We will visit some 1D nanostructured forms of transition metal (TM) MO2 nanotubes and nanorods, showing their particular properties for their possible implementation in state-of-the-art catalytic devices. In this line, motivated by the worlds ever increasing need for cleaner burning fuels and more viable forms of renewable energy, hydrogen production via photocatalysis has been intensely researched as a posible candidate for addressing these issues; for this purpose, N and B doped TiO2 nanorods and nanotubes arise as potentials for their implementation in light-harvesting devices, since the inclussion of a-la-carte dopant mid-gap states permits the tunning of their photoabsorption/emission optical properties, increasing the photocataytic efficiency.

Regarding Molecular Electronics, mechanical properties and electronic transport has been analyzed for Au and Al nanowires. In order to combine both catalytic and transport properties, the effect of protonated (or high H2 content atmosphere) is also analyzed. But not only metal wires show interesting electronic transport properties. Recently, it has been shown that a metallic oxide combination, RuO2/SiO2, consisting of a transparent conductive Pt group metal oxide and a dielectric insulating silica material, can be constructed in a cylindrical layered fashion with enhanced transport properties. First of all, due to the lack of information, we have analyzed both subsystems by separate for a first undestanding of their specific properties before understanding their effective combination. Tunable photoabsorption and photoemission properties will be shown for the case of confined organic molecules inside single-walled carbon nanotubes, to finally conclude with the first theoretical attemp of constructing a molecular transistor based on TM/N-functionalized carbon nanotubes.

All the previous issues have been analyzed within a detailed theoretical framework involving the most advanced theoretical tools, such as many-body perturbation theory for the electronic characterization, and the Keldish-Green / Fisher-Lee formalism for the electronic transport description, and the theoretical scanning tunneling microscopy.

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