

Featuring the *State of the Art of Nanosciences in Belgium*

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1. Introduction

Like in many countries, research devoted to nanosciences in Belgium grew up after high-resolution electron microscopy and local probe microscopic tools became available. The concomitant development of nanostructure fabrication techniques, like CVD, electrodeposition and solgel synthesis, gave a further impulse to the field. Subsequently, the mastering of nanofabrication by lithography and focused ion beam, to cite a few cases, pushed the nanoscience research into its golden age. In parallel, the elaboration of more and more sophisticated ab initio software, together with the constant rise in computer performance, have opened the way to more and more accurate computational tools. Nowadays, it is becoming possible to predict the properties of new nanostructures and nanodevices beforehand. All these aspects of nanoscience research are developed in Belgian universities and research centers. IMEC, one of the largest European research centers for nanosciences and nanoelectronics, is located in Leuven [1].

This special issue is by far not an overview of all of what is going on in the nanosciences under the Belgian banner. This would require thousands of pages. The few documents contained in this special issue will give the readers a flavor of what the development of nanosciences looks like in this country. In the following lines, the papers are briefly presented. They have been grouped into four main topics: (1) Electronic structure and quantum transport, (2) optical and electromagnetic properties, (3) production, applications and toxicity, and (4) functionalization.

2. Electronic Structure and Quantum Transport

The contribution of Champagne et al. [2] is a review of the electronic properties in a broad sense of 2D materials given by ab initio density functional theory and empirical tight-binding methods. The expression “carbon flatland” used in the title is an allusion to a song of the famous Belgian singer Jacques Brel who described in a poetic way the beauty of the North part of Belgium, which is indeed very flat. So are perfect 2D materials sustained by an atomically smooth surface. The paper goes beyond ideal structures, for grain boundaries and heterojunctions are also considered.

First-principle computational techniques based on density functional theory have been used by Houssa et al. [3] to predict the current–voltage characteristics of lateral junctions between graphene and 2H-MoS₂ and also 1T-MoS₂ and 2H-MoS₂. Both systems are examples of conducting–semiconducting 2D heterostructures. Different atomic models for the interface have been constructed, some of which involve bilayer graphene or functionalized 1T-MoS₂ as the conducting material. The aim of these computer simulations was to identify low-contact resistance heterostructures for possible 2D nano-electronic devices.

3. Optical and Electromagnetic Properties

Lobet et al. [4] studied numerically the performances of a perovskite-based photovoltaic cell. The photo-active part is a hybrid structure made of nano-spheres of methylammonium lead triiodide perovskite packed onto a uniform slab of the same material. The geometry of the structure was optimized in order to get the largest absorption of solar radiations between 310 and 800 nm wavelength.

Effective mass approximation combined with the $\vec{k} \cdot \vec{p}$ method was used by Gattuso et al. [5] to predict exciton dynamics in a large assembly of CdSe quantum dot dimers. In close connection with the experiment, they calculated the optical response of the dimer assembly to sequences of femtosecond laser pulses similar to what is used in pump-probe transient absorption spectroscopy.

4. Production, Applications and Toxicity

Vertically aligned nanosheets of WSe₂ were synthesized and characterized by Sierra-Castillo et al. [6]. Using atmospheric pressure CVD for the selenization of W thin films on a sapphire substrate, they developed an efficient and scalable growth technique. The nanosheets produced were demonstrated to be highly crystalline and well oriented, while mixing a minor phase with the most stable 2H polymorph.

Nanowires made of Co, Fe, Ni, Py, and their alloys have interesting magnetic properties reviewed by Piraux [7]. As illustrated in his paper, complex and reproducible structures were obtained by electrodeposition techniques, including core-shell nanowires, multilayered nanowires, and 3D networks of interconnected nanowires. Applications of magnetic nanowires are presented, among which there are magnetotransport, magneto-thermoelectric effects, and spin valves. Interestingly enough, some structures present tunable magnetic properties.

Cuong et al. [8] produced poly (L-lactic acid) (PLLA) nanofibers by electrospinning for energy harvesting applications. Using a battery of characterization techniques, they discovered a considerable improvement in the mechanical and piezoelectric properties of nanofibers annealed above the glass temperature that ensued from a much better crystallinity of the post-annealed samples.

In their contribution, Mederos-Henry et al. [9] describe how the inclusion of different kinds of nanoparticles in a polymer can be exploited for producing nanocomposites presenting a high absorbance for microwaves. Improved electromagnetic shielding effectiveness has been achieved by combining sp² carbon nanostructures and magnetic nanoparticles, especially when resorting to a hierarchical organization of these nano-inclusions.

Having used in vivo and in vitro approaches for many years, Orsi et al. [10] have been conducting research on the toxicity of carbon nanotubes for many years. They have demonstrated that the toxicity of nanotubes strongly depends on their size and shape. The mechanisms responsible for the development of a cancer affecting the mesothelium (malign mesothelioma), which up to now has been mostly due to asbestos exposure, have been investigated in animal models using needle-like nanotubes. The authors have discovered that carbon nanotubes, thanks to the broad range of their physico-chemical characteristics, offer several advantages over asbestos for the understanding and the therapy of mesothelioma.

5. Functionalization

A catalytic process for silylation of multiwall carbon nanotubes was assessed by Detriche et al. [11]. After purification, six kinds of modified nanotubes obtained by diazonium chemistry were subsequently functionalized with a silane derivative using either ZnCl₂ as catalyst or Karstedt's catalyst. The products obtained after each step of the process were characterized by XPS and their solubility in 40 different solvents was determined.

Acosta et al. [12] used low-energy (0.5–2 keV) oxygen ion irradiation to chemically modify the surface of vertically aligned multiwall carbon nanotubes. According to microscopic analysis, the nanotube tips were opened by the incident ions and functionalized. It was demonstrated by

XPS that epoxide, carbonyl and carboxyl functional groups were produced in variable concentration, depending on the ion kinetic energy and irradiation time.

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