VIRTUAL ABSTRACT BOOK – INVITED PAPERS

I.1. Porous semiconductor compounds: obtaining and functionalization with metallic nanostructures for multifunctional applications

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The report will focus on different aspects of pore growth during electrochemical etching in a controlled fashion [1], transition from the porous semiconductor structures to the formation of semiconductor nanowires [2,3], as well as technologies for controlled electrochemical deposition of metal nanostructures into porous semiconductor templates [4].

The obtained metal-semiconductor structures were exploited in a variable capacitance device elaboration with a record capacitance density variation of about 6×10^{-3} pF/V per 1 μm^2 of surface [5]. An IR photodetector based on a single GaAs nanowire with good sensitivity and dynamic characteristics was demonstrated [3]. The fabricated core-shell GaAs/Fe nanowire arrays, along with possibilities to tune the orientation to the substrate surface, showed magnetic anisotropy with respect to the coercivity and the remanence ratio [6,7].

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I.2. Continuous change from monoclinic to ferroelectric orthorhombic HfO_2 by a martensitic-like transition – challenge for nonvolatile memories

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In the last decades a lot of effort has been spent for obtaining lead-free ferroelectric materials at nanoscale for micro- and nano - electronic devices, the ferroelectric orthorhombic HfO_2 (o-HfO_2) being one of the most important. The formation of orthorhombic phase and controlling ferroelectricity in HfO_2 are reported in literature to be strongly dependent on factors as size effect, surface and interface energy, oxygen vacancies, dopant concentration and stress [1,2].

We obtain ferroelectric o-HfO_2 in HfO_2/Ge-HfO_2/HfO_2 3-layer structure deposited by magnetron sputtering and then nanostructured by rapid thermal annealing (RTA) [3]. The o-HfO_2 is formed in Ge NCs-HfO_2 intermediate layer, HfO_2 crystallization and ferroelectric phase formation being significantly influenced by Ge doping and the stress field present in the 3-layer. Therefore, o-HfO_2 is also formed inside the adjacent layers, in the 5 nm regions near the interface in which Ge has diffused. At the surface of cap layer/structure surface, HfO_2 is monoclinic.

A continuous spatial transition (over few atomic layers) from monoclinic to orthorhombic phase was revealed inside single HfO_2 nanocrystals. In our opinion, the crystallization mechanism consists in a martensitic-like transformation of the initially grown tetragonal phase that during RTA transforms in orthorhombic (in regions with remaining stress and in those with Ge dopping), and in monoclinic phase where HfO_2 is relaxed, as at 3-layer surface. These leads to the continuous spatial transition from monoclinic to orthorhombic phase under the influence of Ge-doping and remaining stress. Atomistic calculations support our model.
The ferroelectric behavior is revealed by remanent polarization – voltage hysteresis loops and the total remanent polarization is of 6.5 $\mu C/cm^2$, being comparable to the values reported for thick HfO_2 and large ferroelectric domains.

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I.3.
Numerical simulations as a solution to design the desired optical properties of multilayers thin films

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Ellipsometry is a non-destructive, non-invasive non-contact, very precise, reproducible and very sensitive technique for study the ultra-thin films. Spectroscopic ellipsometry (SE) provides a widely applicable method for determining accurate characterization of optical and electrical transport properties of thin films multilayers structures, in particularly when the multilayer of device structure, is of critical importance to their effective implementation. The difficulty consist to discern between two or more ellipsometric models which both fits well the same data. In the most reported data in literature, the ellispometric models studied are considered enough good if the experimental data of the global refractive index (n) and extinction coefficient (k) fits well with the dispersion curves. Improved models can be constructed however by also comparing the calculated the transmission coefficient from ellipsometry with the experimental values obtained from direct spectrophotometry measurements. This procedure allows to establish in a more accurate way the best dispersion model for each sample. The good correlations obtained between the electrical and optical properties determined experimentally by different techniques and the electrical and optical characteristics obtained by theoretical ellipsometric simulations, indicate that high accurate ellipsometric modelling approach, can give the possibility in the future to predict the appropriate device architecture in function of the desired optical and electrical properties and to reduce hence the experimental tests and the waste of materials in the optimization of multilayers thin films fabrication process.

This paper provide a comprehensive study of the spectroscopic ellipsometric measurements of single oxide films and multi layers thin-film coupled with other direct measurements techniques in order to present a possible method for designing, by numerical simulations, new multilayers architectures with the desired properties.

I.4. Optical properties of spatially-ordered two-dimensional structures of spherical particles in absorbing matrix

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The developed by us statistical method to solve the problem of light scattering and absorption by a short- and long-range ordered monolayer of spherical particles in an unbounded nonabsorbing host medium [1-7] is generalized to a host medium with light absorption. It takes into account multiple scattering of waves, is based on the quasicrystalline approximation (QCA), mean field approximation and the expansion of fields and tensor Green's function in terms of the vector spherical wave functions and has no restrictions on the distance between particles. The method allows one to describe optical properties of a "monolayer of spherical particles in light absorbing matrix" system.

The data for coefficients of coherent transmission and reflection, incoherent scattering, and absorption are presented. Comparison with the data for inverse system (the matrix is made from the material of the particles, and the particles are made from the matrix material) is fulfilled.

The influence of particle and matrix complex refractive indices, particle diameters, their spatial order, and monolayer filling factors on the optical properties of the system is considered. The effect of "extraordinary transmittance" is illustrated for monolayer of spherical nanovoids in the silver matrix.

The results obtained can serve as a basis for solving the inverse problem of light scattering. They can be used to solve the wide range of problems of photonics, optoelectronics, and chemistry: to develop the solar cells, photonic crystals, optical coatings, photodetectors, chemical photoreactors, and other devices based on particulate two-dimensional structures.

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I.5.
Tandem heterojunction solar cells with Cu_2O/ZnO Si based: optimization and defect analysis

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A four-terminal Cu_2O/ c-Si tandem heterojunction solar cell was investigated. The electrical and optical characteristics for aluminium doped ZnO (AZO) and undoped Cu_2O thin film layers were determined.
The modeling of solar device was based on two main simulation softwares: 1) Silvaco used for the top Cu_2O/Zn O subcell, and 2) PC1D/Quokka 2 for the bottom c-Si subcell[1]. Numerical modelling allowed to analyse the main electrical parameters of the two sub cells, in order to optimize the performance of the solar device. A power conversion efficiency of 24.7 % for the four-terminal Cu_2O/c-Si tandem heterojunction solar cell was obtained. The effect of interface defects on the electrical characteristics of the AZO/Cu_2O heterojunction was evaluated. The analysis suggested that the incorporation of a buffer layer could improve the performance of the heterojunction solar cell.

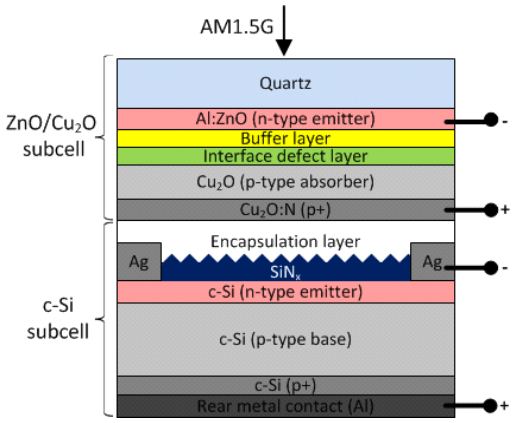

Figure 1. The heterojunction solar cell based on sputtering deposition of metal oxides

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I.6.
DICATIONIC IMIDAZOLIUM AND PYRIDINIUM SALTS: STUDY OF IONIC CONDUCTIVITY, LIQUID CRYSTALLINE AND EMISSION PROPERTIES

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Ionic liquid crystals (ILCs) are a distinct class of materials with unique properties resulting from the combination of liquid crystals and ionic liquids behaviour. ILCs based on imidazolium or pyridinium salts are very well documented; in fact, these salts are the most common ILCs studied for their exceptional characteristics such as low volatility, nonflammability, tunable polarity, high-ionic conductivity related to their ionic liquid nature in connection with their liquid crystalline properties.[1-3] Some recent applications were added: battery materials, solar cells, electrochemical sensors, organic reaction media or electroluminescent switches.

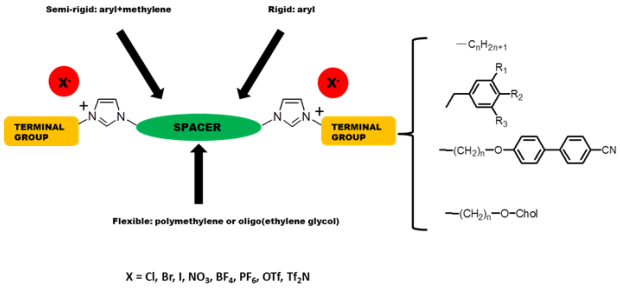

Figure 1. ILCs based on bisimidazolium salts.

This presentation will focus on the design and characterization of various dicationic ionic liquid crystals based on imidazolium or pyiridinium salts with various counterions, which have been reported recently by our group. The type of mesogenic group, spacer length and the nature of counterion will be related to the liquid crystals properties. Also, the emission properties of the simple organic salt or coupled with emissive units (polyoxometalates) will be discussed.

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I.7. PCM simple modelling and energy storage simulation

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Nowadays efforts are made to develop more efficient techniques for producing electric energy from renewable energy sources. In this context, a special attention is directed towards the solar to electric energy conversion. This can be obtained either directly by employing photovoltaic panels, or indirectly by using thermodynamic cycles. One main advantage of the last methods consists in the possibility of extending the system operation over periods of solar energy unavailability, by integrating a thermal energy storage subsystem. Phase change materials (PCM) turn out to be good candidates for such purposes.

The proposed paper provides a simple mathematical modelling, based on energy conservation law, to simulate the melting process of a PCM driven a commercial parabolic through collector (PTC). The considered system is presented in Figure 1.

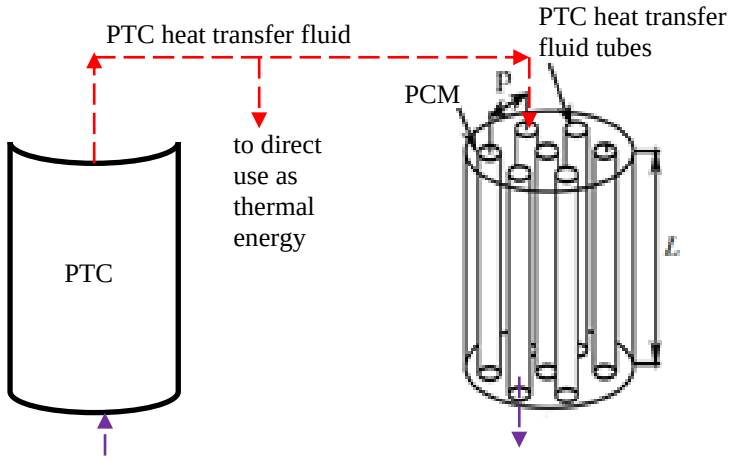

Figure 1. PTC-PCM studied system.

Analytical development, as well as numerical and graphical results are presented for several days operation. Sensitivity studies with respect to system dimension (number of coupled PTC and PCM modules) are included.

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I.8. Adsorption of Methylene Blue upon substrates of fabrics and filter paper type

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We have recently investigated the photocatalytic behavior of some fabrics deposited with semiconductor oxide (TiO2, ZnO) nanoparticles in pure or doped state; methylene blue (MB) and its degradation was chosen as a well known dye and test reaction (see e.g. [1,2] and the long list of reference cited herein). Closely related to these, is the radial liquid spreading from an infinite reservoir containing a dye solution onto a horizontal fabric or a common filter paper (which are playing as the catalyst supports): The topic is discussed in this presentation.
The images of the wet spot during the radial wicking were collected with a webcam; then these were processed with routines giving the area of the wet spot as function of time. One can thus speak about the wicking kinetics and further, about the possible mechanism. The experiments were performed using polyester (PES) and wool (WO) samples differing not only by the yarn composition but also by the roughness of the surfaces. White or colored fabrics were considered The data were compared with the results obtained for the common filter paper (CFP) for laboratory use.
MB was commercially purchased and used as such. Aqueous MB solutions were either diluted (0.1 mM) or more concentrated (1 mM). Sample notation keeps the material label for the 'substrate' while MB appears with the dye concentration; thus MB(0.1)/CFP means a filter paper sample imbibed with diluted MB solution.
The samples were routinely characterized both in the original and the MB deposited form as well to consider the structure, the surface morphology and the deposition changes. by applying several techniques [1,2].
MB wicking in textiles was followed by an optical method. The analysis of the images of the wet spots allows to conclude that the procedure developed is useful in comparing the behavior of the fabrics against the MB imbibition and further in the tests of MB degradation. Moreover, the kinetics of wetting can be discussed as well. There are elliptical wet spots. Water (the solvent) has a higher wicking rate than the dye. The dye is concentrated in a small region due to adsorption upon supports. The evolution of the elliptical wet spot conserves the ratio of the main ellipse axes.
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I.9.
At the Frontier Between Materials Science and Biotechnology: Nanomaterials Phytosynthesis

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Nanotechnology represents one of the most important advances in materials science, as it provided important break-throughs in many different aspects of every day life. Among different methods for nanomaterials development, phytosynthesis of materials is of part importance due to its several advantages of other methods.

For over a decade now, our research group evaluated the possibilities of phytosynthesis of different types of nanoparticles, gaining insights on the advantages of this method, as well as on its limitations. A successful approach for the development of phytosynthesized nanomaterials with enhanced applications requires an application-correlated strategy, involving knowledge of biotechnology, nanotechnology, materials science and others.

Through selected examples from our published works [1-3], the high potential of the phytosynthesized nanomaterials for practical applications will be clearly demonstrated.

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I.10. Pincer Complexes of Gold(III): Organometallic Chemistry, Liquid Crystals, Photophysics and OLEDs

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Gold(III) complexes of *C^N^C* pincer ligand are promising emissive materials for OLED devices owing to the accessibility of triplet excited states. It is likely that there is also merit in further functionalising the emissive component of OLEDs by conferring liquid crystal properties and, to that end, we undertook the preparation of several series of materials with the general structure shown in the Figure.

The complexes vary through: (i) the number/position(s) of chains on the pincer backbone (*n* = 1 or 2) and (ii) the number and nature of the chains (hydrocarbon and semiperfluorocarbon) on the phenyl-acetylene (*m* = 0-3).

Among the properties are: (i) good photoluminescence quantum yields and OLED external quantum efficiencies; [1] (ii) wide-range liquid crystal mesophases

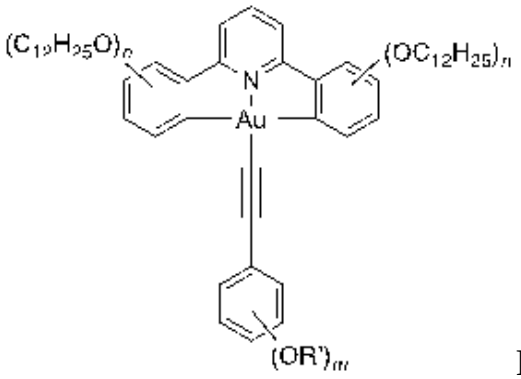

Figure: General structure of the complexes investigated in this study.

[1,2] and (iii) almost unprecedented observation of a frustrated nematic liquid crystal phase in a disc-like material.[3] Furthermore, such complexes cannot be synthesised directly from the ligand, rather through a toxic intermediate organomercury(II). Importantly we have recently shown how they can now be accessed either through palladium(II) intermediates or directly using Rh catalysis. [4]

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