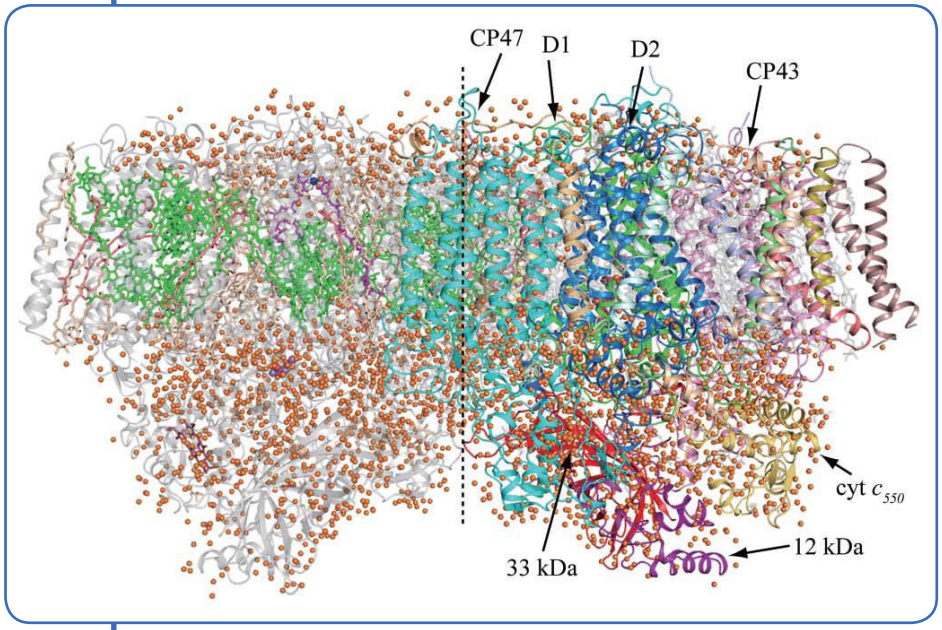
Advanced workshop on
solar energy conversion

Abstracts



21-23 May 2012, Bucharest, Romania

The workshop is organized by:

- UNESCO Chair on Sustainable Development at Horia Hulubei Foundation (Magurele-Bucharest)
- National Institute for Materials Science (Magurele-Bucharest)
- Faculty of Physics, University of Bucharest
- Abdus Salam International Centre of Theoretical Physics (Trieste)
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Notes

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Program

May 21

9.30 – 9.50: Opening remarks, Stefan ANTOHE and Joseph NIEMELA
9.50 – 10.20: Eric Daniel GLOVACKI: Learning from nature: hydrogen-bonded macromolecules for organic electronics
10.20 – 11.00: Paolo FORNASIERO: Photocatalitic H_2 and added value byproducts: the role of metal oxide systems in their synthesis from liquid oxygenates
11.00 – 11.10: Coffee break
11.10 – 12.10: Vanni LUGHI: Nanotechnology for photovoltaics
12.10 – 12.50: Leonid CULIUC: Preparation of solar cells by low cost spraying technology

12.50 – 15.00: Lunch break

15.00 – 15.45: Stefan ANTOHE: Polymer/Fullerene bulk heterojunctions and inorganic/organic hybrid structures for photovoltaic applications
15.45 – 16.30: Gabriel SOCOL: Materials for photovoltaic applications prepared by pulsed laser deposition
16.30 – 16.45: Coffee break
16.45 – 17.30: Eugenia FAGADAR-COSMA: New hybrid nanomaterials based on silica-porphyrin
17.30 – 18.15: Monica ENCULESCU: Nanomaterials with taylored properties by template and templateless approaches for photovoltaic applications
18.15 – 19.00: Mihai GIRTU: Dye-sensitized solar cells – a combined experimental and theoretical approach

19.30: Welcome party

May 22

9.30 – 10.15: Paolo FORNASIERO: Exceptional activity for methane oxidation with catalysts prepared by modular assembly of Pd@CeO2 subunits
10.15 – 11.15: Stefano FABRIS: Computational modeling of new materials for solar-driven fuel production
11.15 – 11.30: Coffee break
11.30 – 12.30: Nicola SERIANI: Computational materials science for energy applications

12.40 – 15.00: Lunch break

15.00 – 15.45: Teketel Yohannes ANSHEBO: Conducting polymers based photo-electrochemical solar energy conversion
15.45 – 16.25: Magdalena NISTOR: Transparent conductors obtained by pulsed electron deposition
16.25 – 16.35: Coffee break
16.35 – 17.20: Branko PIVAC: Nanomaterials for photovoltaics
17.20 – 17.50: Petre PALADE: Hydrogen storage materials
17.50 – 18.30: Mihaela GIRTAN: Electronics and photonics: two sciences in the benefit of solar energy conversion

18.30 – 19.30: Poster session

May 23

9.30 – 10.15: Daniel EGBE: Polymer-based organic solar cells
10.15 – 11.15: Serdar SARICIFTCI: Organic-inorganic nanostructures for solar energy conversion
11.15 – 11.30: Coffee break
11.30 – 12.30: Serdar SARICIFTCI: Charge carrier transport in organic photovoltaic devices
12.30 – 12.45: Daniel EGBE: ANSOLE – solar energy for Africa
12.45 – 13.15: Discussions and perspectives

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POLYMER/FULLERENE BULK HETEROJUNCTIONS AND INORGANIC/ ORGANIC HYBRID STRUCTURES FOR PHOTOVOLTAIC APPLICATIONS

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In the last decades the third and forth generations of photovoltaic cells based both on the organic thin films and hybrid nanostructured inorganic/organic materials structures have attracted a great deal of interest due to the low-cost of organic materials, their origin from non-toxic precursors and the simplicity of producing technologies. Among the organic semiconductors envisaged to be used in such structures, the small molecules like metal-doped phthalocyanines and polymers are the most studied. Their optical absorption in the visible range of the solar spectrum is strong, but based on an excitonic mechanism. A typical value for the diffusion length of the exciton in organic semiconductors is of 20-80 nm, while in order to achieve the required efficiency in light absorption, the absorber layer has to be at least 100 nm thick. One way to improve the extraction of the charge carriers will consist in significantly increasing of the area of the interface between the two components of the heterostructure, expecting to take place in the third and fourth generation of solar cells.

In this work are summarized the electrical and photoelectrical properties of the organic photovoltaic cells based on the polymeric thin films and hybrid inorganic/ organic structures.

In the case of third generation of solar cells, the polymer (P3HT, PCBM or MEH-PPV, PCBM and their blend, respectively) based photovoltaic cells were produced by spin-coating technique. The structures based on the P3HT: PCBM (1:1) or MEH-PPV:PCBM(1:4) blend shows a promising photovoltaic response, with a power conversion efficiency increased of about two order of degree, with respect of those measured in the case of structures based on a single polymer used as photoactive layer. Such as above shown, one way to improve the extraction of the charge carriers will consist in significantly increasing of the area of the interface between the two components of the heterostructure, then reducing the dimensions of D/A heterojunctions to the dimension of exciton diffusion length in the organic absorber. In this way the driving forces, due to potential difference between Donor LUMO and Acceptor LUMO, will acts efficiently for exciton dissociation and photo charge carrier generation in photovoltaic cells based on polymeric blends.

The same idea is used in the case of fourth generation solar cells where a nanostructured inorganic thin film is sensitized with a good organic absorber, generally a dye leading to solid Dye Sensitized Solar Cells.

In this case we report two kind of prepared and characterized structures: i) hybrid

structures based on nanostructured ZnO electrode, photosensitized by CuPC; ii) hybrid structures based on CdTe nanowires arrays/ZnPc or TPyP.

Three types of hybrid structures based on nanostructured ZnO were prepared: a) Nanostructured ZnO thin films/CuPc; b) ZnO nanowires array/CuPc; c) ZnO nanotubes array/CuPc. EQE of ZnO wire arrays/CuPc structures was 4 time larger than that of ZnO nanostructured film/CuPc structures and EQE of ZnO nanotubes arrays/CuPc structures was about one order of magnitude higher than that of ZnO nanostructured film/CuPc structures.

For second type, hybrid cells based on the heterostructure at the interface between wire arrays of CdTe, and the organic film ZnPc and TPyP, were produced and characterized. EQE of CdTe nws/CdTe (200nm)/ZnPc structures was two order of magnitude higher than in the case of CdTe nws/ZnPc.

Currently, work is in progress to improve the efficiency of these structures, by optimizing the density of the nanowire or nanotube arrays, and improving the quality of the inorganic/organic interfaces.

Keywords: *nanostructured materials for photovoltaic applications „Bulk Heterojunction" photovoltaic cells, hybrid inorganic/organic photovoltaic cells*

PREPARATION OF SOLAR CELLS BY LOW COST SPRAYING TECHNOLOGY

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The main semiconductor material for solar cells (SC) and modules fabrication is silicon. The production of silicon SC is largely developed in the world, but the principal obstacle in such SC utilization, especially in developing countries, is their relatively high cost.The SC price reduction can be obtained by utilization of low cost fabrication technologies. The pyrolithical spraying method, which permits to obtain semiconductor-insulator-semiconductor (SIS) structures, is an example of such technology. This method has some advantages, the most important of them being the simplicity of barrier structure obtaining. This technology needs considerably lower temperatures, no more than 500°C, and shorter time that in the case of p-n junction fabrication by diffusion processes. Besides Si, other solar semiconductor materials such as InP CdTe, GaAs have been also used for SIS type SC preparation.

ITO thin films have been obtained using two variants of spray deposition. The first variant was described in [1] and is characterized by direct spraying of the diffused flux of the drops of the alcoholic solution of the mixture of indium and tin chlorides on the

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surface of single crystalline Si wafers. This surface can be smooth or texturized. The second variant of the deposition process, named indirect spraying, differs from the first one. In the second case, the flux of solution drops does not directly hit the silicon surface, but, first, passes through a glass tube supplied with a labyrinth of obstacles, which favours a more intense dispersion of the solution drops. Hence, rather a flux of solution vapours is formed on the substrate surface but not a flux of dispersed drops. In addition, the speed of the vapour flux can be controlled in a wide range of values.

ITO thin films with the thickness 280-300nm were obtained on the smooth surface of Si single crystals by direct spraying at the compressed air pressure of 0.5 atm, using 12 ml of the solution, whereas at indirect spraying, for the same quantity of solution and air pressure of 0.1 atm, the ITO thin films thickness is 660-700nm.

In both cases the layer consists of crystallites in the form of parallelepipeds with tetrahedral pyramids in peaks. Crystallites grow perpendicularly to (100) oriented silicon surface. If texturized Si substrates are used (inverted pyramids obtained by photolithography) ITO layer deposited by direct spraying evenly covers the surface. Indirect spraying provides full coverage by ITO of the texturized silicon surface, but the coverage is uneven - thicker outside of pyramids and thinner within them. ITO thin layers obtained by spray technique on the (100) surface of silicon wafers are polycrystalline. Tetrahedrally shaped crystallites grow perpendicular to the substrate plane, their height is comparable to the thickness of the layer, and the side width reaches the values ~ 200x200nm for indirect spraying of the chemical solution of indium and tin chlorides.

The above mentioned method of SC preparation has been used for obtaining mono- and bifacial SC. To be more precise, on the base of ITO layers deposited on the texturized surface of Si wafers, formed by inverted pyramids, ITO/Si structures and Ag/n^+ITO/SiO_2/nSi/n^+Si/Ag solar cells have been obtained with the record efficiencies of 15% for this type of solar cells.

Two types of bifacial SC, which have different profiles of silicon wafer surface, have been also obtained. The effected technology optimization allows increasing the resultant efficiency from 13.9% [2] to 15.73% in the case of irregular etching of the silicon surface and up to 20.89 % in the case of regular etching. The bifaciality ratio is also increasing from 0.38 up to 07.

In such a way a novel type of bifacial cells containing only isotype junctions was elaborated. Their advantages are the following: the frontal junction is obtained with a simple spray technique at low temperatures; the frontal ITO layer is a collecting electrode and, at the same time, an antireflection coating.

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POLYMER-BASED ORGANIC SOLAR CELLS: EFFICIENT TUNING OF ACTIVE LAYER NANOMORPHOLOGY USING ALKOXY SIDE

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Alkoxy side chains grafted on the backbone of conjugated polymers have primarily a solubilizing function; they enable the processability of conjugated materials into thin films for various optoelectronic applications. Beyond this primary function, alkoxy side chains strongly influence the supramolecular ordering of the polymers in solid state, which consequently has an impact on the thermal behavior and the physicochemical properties of such photoactive materials.[1-3]

Using poly(arylene-ethynylene)-*alt*-poly(arylene-vinylene)s, **PAE-PAV**s, a new class of conjugated materials combining the interesting intrinsic properties of both poly(arylene-ethynylene)s (**PAE**s) and poly(arylene-vinylene)s (**PAV**s), we were able to demonstrate that the hydrophobic nature of alkoxy side groups can be used to tune the solar cells active layer nanomorphology. The bulk heterojunction intermixing between donor (polymer) and acceptor (fullerene derivative) was shown to be significantly dependent on the side chains nature (linear and/or branched) and volume fraction. Systematic side chain fine tuning has led to an increase of the energy conversion efficiency, $\eta_{AM1.5,}$ from 0.3% to 5.0%, the latter value being the present state-of-the-art efficiency for **PAV** based materials.[4-8]

Keywords: *Organic solar cells, alkoxy side chains, polymers, nanomorphology.*

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COMPUTATIONAL MODELING OF NEW MATERIALS FOR SOLAR-DRIVEN FUEL PRODUCTION

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The conversion and storage of solar energy into chemical fuels rely on finding novel catalytic materials for the electrochemical splitting of water. These catalysts should be stable, inexpensive, efficient and easily integrable in photovoltaic units. In this talk I will present an overview of how state-of-the-art computational modeling can provide the missing insight into the structure and function of some of the most promising candidate anodic materials for artificial leaf technologies.

In particular I will address three paradigmatic water-oxidation class of catalysts: i) Heterogeneous amorphous cobalt-phosphate nanoparticles based on earth-abundant elements [1]; ii) Homogeneous molecular complexes, both organic and inorganic, based on single and multiple metal centers[2-4]; and iii) hybrid nanostructures consisting of molecular catalysts bound to functionalized conducting substrates [5]. The calculated results [6-9] allow for rationalizing the available experimental data and identify the origins of the high reactivity and stability of these novel catalysts.

* The work is done in collaboration with Simone Piccinin, Changru Ma, Xiao Liang Hu, and Alessandro Laio.

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FROM TAILORING PORPHYRINS TO ADVANCED OPTOELECTRONICS NANOMATERIALS

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Porphyrins are characterized by a rich self-assembly chemistry and therefore they offer the possibility to grow and generate Self-Assembled Nanoparticles in one step, and as function of their designed amphifilic structure can influence the size and shape of the nanoparticles, but also arrange them into highly organized nanostructures.

Tailoring porphyrins by modifying the substitution in meso-aryl groups with pyridyl, carboxyl or hydroxyl confers some degree of hydrophilicity and may cause a bathochromic shift-moving Q Band to red and this was a start to find an innovative formulation for photosensitizers [1].

New series of differentially functionalized porphyrins was obtained by a multicomponent synthesis (adapted Adler-Longo method) by simultaneously using of two different aldehydes. By using proper stoichiometry of the reagents, this type of reaction is often used for the preparation of porphyrinsA_3B type containing three substituted phenyl rings derived from one aldehyde and one substituted phenyl ring derived from the other [2].

The purified porphyrins were characterized by HPLC, TLC, FT-IR, UV-vis, fluorescence, MS, XRD and NMR analysis. Thermal analysis and AFM was also performed. All the obtained porphyrins belong to second generation asymmetrical meso-tetraphenylporphyrins, having the capacity to absorb at long wave length in the red region of the visible spectrum ($\lambda > 630$ nm).

Novel porphyrin-silica nanomaterials have been prepared by using different approaches of controlled sol-gel process: in situ, by impregnation and by sonication, via one step acid and two steps acid-base catalyzed hydrolysis and condensation of different mixtures of silica precursors. The materials obtained by one step acid catalyzed sol-gel procedure exhibit a very important bathochromic and hyperchromic shift in the red region, towards 720 nm, that makes them promising second generation photosensitizers [3-6]. AFM images of the synthesized nanomaterials display tuned particles of ultralow size (40-70 nm) controlled shape and high porosity. Stacking generates various shapes from convex-concave supramolecules to some pyramidal nanostructures or even rings and tubes.

Another goal of our research is to investigate the coupling of gold and silver nanoparticles (GNP and AgNP) with different porphyrins molecules. The exchange of the initial ligand (citrate ions) with porphyrins formed hybrid nanostructures (35-40 nm) and change the electronic properties of GNP and AgNP. The pH value has

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a great importance in the coupling of nanoparticles and porphyrins. The effect of porphyrin dye molecules on the plasmon properties of nanoparticles was demonstrated by UV-Vis, fluorescence and electrochemical spectroscopy (OTTLE cell). These new hybrid materials will be also helpful for the design of light harvesting cells [7] and sensors.

The newly obtained A_3B porphyrins were also used as ionophores for preparing PVC-based membrane sensors selective to iron(III). The membranes have the composition: ionophore: PVC: *o*-nitrophenyloctylether (plasticizer) in the ratio 1:33:66. Sodiumtetraphenylborate was used as additive (20 mol.% relative to ionophore). The performance characteristics (linear concentration range, slope and selectivity) of the sensors were investigated. The best results were obtained for the membrane based on 5-(4-carboxyphenyl)-5,10,15-tris(4-phenoxyphenyl)-porphyrin, in a linear range from $1x10^{-7}$ – $1x10^{-2}$ M with a slope of 21.8 mV/decade. The electrode showed high selectivity with respect to alkaline, alkaline earth, and heavy metal ions and a response time of 20 s. The influence of pH on the sensor response was studied. The sensor was used for a period of two months and the utility has been tested for the quantitative determination of Fe(III) in recovered solutions from spent lithium ion batteries*.

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Keywords: *Porphyrins, second-generation photosentisizers, hybrid organic-inorganic nanomaterials, metal sensors, recycling Li batteries.*

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EXCEPTIONAL ACTIVITY FOR METHANE OXIDATION WITH CATALYSTS PREPARED BY MODULAR ASSEMBLY OF Pd@CeO2 SUBUNITS

M. Cargnello, J. J. Delgado Jaén, J. C. Hernández Garrido, K. Bakhmutsky, T. Montini, J. J. Calvino Gamez, R. J. Gorte, P. Fornasiero

There is a critical need for improved methane-oxidation catalysts to both reduce emissions of methane, a green-house gas that will soon be regulated, and significantly enhance the efficiency of power generation in gas turbines. However, materials that are currently available either perform poorly below 400°C or are unstable at higher temperatures. Here, we describe an entirely new approach in which single units composed of a Pd core and a CeO_2 shell are pre-organized in solution and then homogeneously deposited onto a modified hydrophobic alumina. Enhanced metal support interactions lead to exceptionally high methane oxidation activity, with complete conversion below 400°C and outstanding thermal stability under demanding conditions. This work demonstrates that a supramolecular approach can provide a powerful new strategy for high-performance catalytic materials.

NANOMATERIALS WITH TAILORED PROPERTIES BY TEMPLATE AND TEMPLATELESS APPROACHES FOR PHOTOVOLTAICS

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PHOTOCATALYTIC H_2 AND ADDED-VALUE BYPRODUCTS: THE ROLE OF METAL OXIDE SYSTEMS IN THEIR SYNTHESIS FROM LIQUID OXYGENATES

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The growing demand for hydrogen for industrial use and as a fuel pushes for innovative and sustainable production strategies, which can be applied both in centralized, large-scale plants and in delocalized small units. An attractive option is the photocatalytic reforming of oxygenate / biomass-derived compounds. In fact, upon photoactivation in the presence of an appropriate semiconductor, such feedstocks can undergo oxidation to CO_2 with simultaneous H_2 production. However, when the oxidation is selective rather than complete, the process might be of further

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interest due to the added value of the obtained carbon-containing by-products. In this respect, there is a growing interest in the exploitation of representative biomass-derived oxygenated compounds, such as methanol, ethanol, glycerol, and sugars.

ELECTRONICS AND PHOTONICS: TWO SCIENCES IN THE BENEFIT OF SOLAR ENERGY CONVERSION

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This talk gives a global point of view on two sciences: Electronics and Photonics towards the solar energy conversion. The new research directions in these two sciences are pointed out in connection with the renewable energies. Building with sand…. The human being intelligence transformed the sand in buildings, glass, optical fibers, computers, solar cells etc. One of the most abundant chemical compounds in nature is the silicon dioxide, also known as silica. Silica is most commonly found in nature in sand or quartz. Silicon is prepared starting from silica and quite the whole electronics today is based on silicon. Photonics is based fundamentally on silicon dioxide (glasses, optical fibers, lenses). So finally the whole world today based on electronics and photonics, with computers, optical transmission data, mobile phones, solar cells, use sand as starting material. Of course there are other elements and sand alone couldn't be use to get all these ends. Beside inorganic materials, the new research achievements show that organic materials could be also used successfully for electronics and photonics. The new trends in physics and technology are the plastic electronics and plastic photonics. Most recent studies proved that in the next future the sand will be replaced by graphene. This talk presents a parallel and the equivalence between the electronics and photonics. Starting from electron in electronics, photon, solitons and plasmons in photonics, electrical cables – optical fibers, plasmonic wave guides, electrical circuits - optical circuits, electrical transistors – optical transistors, plasmonster, electrical generators – pulsed lasers and spasers, photonics gets step by step all the tools already existing in electronics. Solar energy could be converted in many ways, the most known is the conversion in electricity. Today we need that the energy is in form of electricity because most of the apparatus that we use are based on electricity: informatics, motors. However the progress in photonics with optical circuits, optical transistors, etc shows that the photonics informatics will be possible. Also the optical manipulation and optical engines concept were already demonstrated experimentally. If the laser propulsion will be achieved, and the optical engines will work, the question that will rise tomorrow is "Shall we still use the electricity in the future ? What will be the solar devices tomorrow ?"

DYE-SENSITIZED SOLAR CELLS – A COMBINED EXPERIMENTAL AND THEORETICAL APPROACH

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We report results of combined experimental and theoretical studies of metal-free dyes used as sensitizers for TiO_2 dye-sensitized solar cells (DSSCs). To analyze the compliance of the various pigments with the main criteria [1] that should be met by a dye to be used as TiO_2 sensitizer in a DSSCs, we performed Density Functional Theory calculations, which provided the optimized geometry, electronic structure and electronic spectrum of the dyes in fully protonated as well as partially deprotonated forms, in solution. For each dye we discuss the adsorption onto the substrate, the matching of the absorption spectrum of the dye with the solar spectrum, the energy level alignment with the semiconductor and the electrolyte [2], and the charge transfer to the substrate. Examples of dyes used include 5-(4-sulfophenylazo) salicylic acid disodium salt, known as Mordant Yellow 10 [3], four azodyes derived from different heterocyclic systems [4], and various natural pigments based on antocyanins [5] and betalains [6]. By comparing the theoretical results with the experimental data, referring particularly to the photovoltaic conversion efficiency, fill factor, short-circuit current and open-circuit voltage, measured under standard AM1.5 conditions, we discuss the importance of these criteria and identify the dyes that meet such requirements.

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PHOTOVOLTAIV PROPERTIES OF SOLAR mc-Si GROWN BY 3D INDUSTRIAL PROCESS

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SYMMETRIZATION OF THE EQUATIONS OF ELECTROMAGNETIC FIELD THEORY - PROPAGATION IN ANISOTROPIC MEDIA

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The propagation of electromagnetic waves in isotropic and anisotropic matter is examined taking into account the symmetrization of equations of electromagnetic field. Along with scalar and vector potentials of electromagnetic field new auxiliary values are introduced: scalar and vector currents. According to these transformations, the Maxwell equation turns into the D`Alembert ones written for anisotropic case. The obtained results are new and interesting.

Keywords: *symmetrization, equation, potentials, anisotropy*

CHARACTERIZATION OF CdTe SOLAR CELLS WITH DIFFERENT WINDOWS LAYERS

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This presentation will focus on characterization of the heterojuntion thin film solar cells based on CdTe. ZnSe/CdTe and CdS/CdTe thin film heterojunction solar cells were fabricated by close Space Sublimation (CSS) on TCO-coated glass substrates. All types of solar cells were fabricated in a superstrate configuration. The thickness of ZnSe and CdS layers was varied in order to adjust the solar cell performance. A cadmium chloride solution for the treatment of a CdTe layer with an elevated temperature air annealing of the completed devices before the back contact deposition was applied to ZnSe/CdTe and CdS/CdTe thin film heterojunctions solar cells. All cells were characterized through light and dark current density-voltage (J-V), capacitance-voltage (C-V) measurements and quantum efficiency (QE) measurements. The saturation current, ideality factor, the depletion width, the charge density distribution across the depletion region and photovoltaic parameters for all thin film heterojunction solar cells will be presented. The investigation at the room temperature under illumination of 100 mW/cm2 through the wide gap components of ZnSe/CdTe and CdS/CdTe heterojunctions showed a value of conversion efficiency (ç) of solar energy to electric energy about 7% and 10.5%, respectively. The incorporation of Zn at the ZnSe and CdTe interface doubles the short circuit current density and improves the performance of ZnSe/CdTe thin film heterojunction solar cells.

Keywords: *ZnSe, CdS, CdTe Thin Films, Close Spaced Sublimation Method, Thin Film Heterojunction Solar Cells*

LEARNING FROM NATURE: HYDROGEN-BONDED MOLECULES FOR ORGANIC ELECTRONICS

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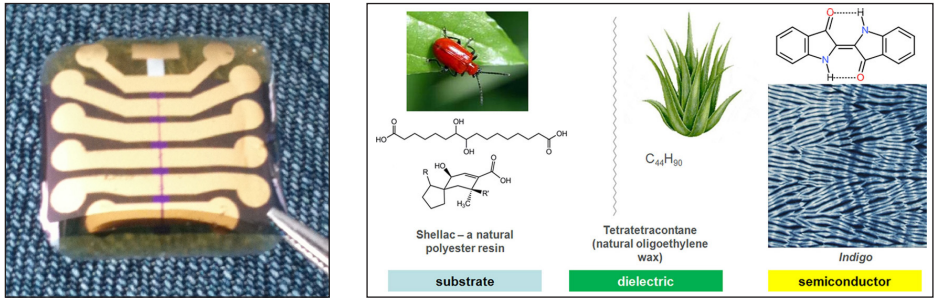
Many natural chromophores feature intra- and inter-molecular hydrogen bonding. Our motivation for exploring such molecules is the realization of biodegradable and biocompatible electronics fabricated from cheap and nontoxic materials. We find that dye molecules such as indigo, tyrian purple, and quinacridones form highly-ordered thin films with excellent π-stacking along one crystallographic axis. Using such films, we have demonstrated field-effect transistors and complementary-like circuit elements utilizing exclusively natural materials operating at the state-of-the-art level with respect to mobility and operational stability in ambient conditions. These dyes show air-stable ambipolar charge transport with balanced hole and electron mobilities in the range of 1×10^{-2} – 2 cm^2/Vs. Such performance places these molecules among the best organic semiconducting molecules reported to-date. Hydrogen-bonding causes strong intermolecular electronic coupling, resulting in optical properties dominated by excimeric and charge-transfer effects. We exploit these properties to fabricate single-layer metal-insulator-metal solar cell diodes that show high photocurrent yields usually thought to be accessible only with the use of donor-acceptor heterojunctions. Hydrogen-bonded natural and nature-inspired materials are an interesting and previously unexplored class of organic semiconductors. In this talk, I will discuss what we can learn about molecular semiconductor design from these fascinating molecules.



An example of thin-film indigo transistors fabricated from natural materials. A photo of the finished devices is shown on the left, while the schematic of materials from substrate, dielectric, to semiconductor is shown on the right.

NANOTECHNOLOGY FOR PHOTOVOLTAICS

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The state of the art of photovoltaics will be reviewed, identifying the fundamental limitations of current approaches and how research on "third generation" technologies is trying to overcome such limitations. All new approaches are based on engineering devices and materials at the nanoscale, as this is the scale where the key mechanisms that govern the photovoltaic effect operate: nanotechnology and biotechnology are the tools of choice for such endeavor. Among such approaches, I will emphasize the contribution of our group at the University of Trieste - focused on a novel class of photovoltaic nanostructured materials obtained from low-cost colloidal chemistry.

TRANSPARENT CONDUCTORS OBTAINED BY PULSED ELECTRON DEPOSITION

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HYDROGEN STORAGE MATERIALS

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NARROW GAP DILUTED MAGNETIC SEMICONDUCTORS FOR OPTOELECTRONIC DEVICES

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THE INFLUENCE OF ZnO NANOPARTICLES ON THE PHOTOVOLTAIC PERFORMANCES OF STRUCTURED BASED ON POLYMERIC BLENDS

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Organic photovoltaic cells based on MEH-PPV:PCBM(1:4) were prepared by spin-coating technique on both optical glass and flexible substrates. The goal of this study is to observe how ZnO nanoparticles mixed in PEDOT:PSS solution influence the photovoltaic performances of the prepared samples. The ZnO nanoparticles amount was varied between 0.1 and 0.3 mg and the obtained results for the "customized" structures were compared with those for the "classical" ITO/PEDOT:PSS/MEH-PPV:PCBM(1:4)/LiF/Al. For all samples were drawn the current-voiltage (I-V) characteristics, both in dark and under illumination. Moreover, the action spectra were recorded and the external quantum efficiencies were calculated. To extract the parameters characterizing such devices, the current-voltage characteristics in fourth quadrant were accomplished in AM 1.5 conditions. All actions were performed at room temperature. Photoelectrical measurements indicate that the ZnO nanoparticles have a positive influence on the conversion efficiency, reducing the serial resistance of the structure and improving the stability of the cells.

Keywords: *polymeric blends, ZnO nanoparticles, photovoltaic cells*

EFFECTS OF IONIZING RADIATIONS ON THE PERFORMANCES OF CdS/CdTe PHOTOVOLTAIC CELLS USED IN SPACE APPLICATIONS

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Polycrystalline thin films such as CdS and CdTe continues to be a leading materials for the efficient and low cost solar cells, used both for therestrial and space applications. With a direct bandgap (~ 1.5 eV) close to the ideal photovoltaic conversion efficiency, CdTe is able to absorb a significant fraction of the solar spectrum under AM0 and AM1.5 conditions. However, the efficiencies for the solar energy conversion and their stability, when are used in space applications are still relatively low. That is why, in this paper we study the effects of the high-energy protons and alpha particles irradiation, on the photovoltaic performances of the CdS/CdTe heterojunction solar cells.

The photovoltaic cells were developed on different TCO materials coated optical glass substrates, by conventional thermal vacuum evaporation technique. The CdS/CdTe is given a chemical CdCl2 treatment which enables grain enhancement, reduces the defect density in the films, promotes the interdiffusion of the CdTe and CdS layers and thereby improves solar cell efficiency. From the I-V characteristics in fourth quadrant, at illumination in A.M. 1.5 conditions, the typical parameters as photoelement (short-circuit current, open-circuit voltage, fill factor, power conversion efficiency), were determined and the effect of ionizing radiations on their values was disscussed. It was found that proton irradiation results mainly in the introduction of defects at the CdS/CdTe interface.

Keywords: *photovoltaic cells, proton irradiation, alpha particle, cadmium telluride, thin films*

NANOMATERIALS FOR PHOTOVOLTAICS

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To modify materials and to produce devices suitable for solar energy conversion it was necessary to change and adapt material properties on the microscopic and macroscopic scale. This was realized since long and the first solution was manipulation with defects in material known as defect engineering. This approach was vastly used in development of the solar cells of the first and second generation. Here we shall briefly review this concept.

Recently however, a new approach is developed based on quantum confinement of materials giving a way to new generation of devices and hence solar cells.

We shall see that space confinement at a nanoscale is a new dominant effect bringing the new concepts, and developing new fields like nanoscience and nanotechnology.

The properties of nanoparticles (mostly silicon) embedded in suitable dielectric matrix (oxide, nitride, carbide) have been extensively studied since the discovery of visible light emission in nanocrystals. Experimental and theoretical studies have been performed in order to explain the physical mechanisms related to the light emission from such nanostructures (called quantum dots-QDs), but results are still subject of a debate.

To build a device based on such concepts one will face several difficulties which have to be cleared yet.

In this lecture we shall review some data on this subject to illustrate the problem we are facing in this filed. We shall see the concepts how to build semiconductor QD and how to control it. Structural and optical properties will be shown and discussed. Finally, the most important concept for a device, i.e. its transport properties will be discussed. Here we shall also introduce the percolation phenomenon and the importance of the interfaces. We shall describe some less often used techniques like SAXS and DLTS.

ORGANOMETALLIC MATERIALS FOR LOW ENERGY CONSUMPTION

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CHARGE CARRIER TRANSPORT IN ORGANIC PHOTOVOLTAICS DEVICES

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Organic photovoltaic diodes (OPVDs) and organic solar cells are based on disordered organic semiconductors. The transport is limited due to the localization process. We will give a didactical overview of the different aspects on charge carrier transport, bringing the experimental data and theoretical models into a critical discussion. The improvement of charge carrier mobility will increase the efficiency of organic solar cells.

ORGANIC-INORGANIC NANOSTRUCTURES FOR SOLAR ENERGY CONVERSION

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Organic photovoltaic diodes (OPVDs) and organic solar cells are reviewed. The different energy and electron transfer mechanisms of solar energy harvesting, and as well as conversion, are discussed. Pure organic nanostructures and organic/inorganic hybrid nanostructures are comparatively studied for photovoltaic devices. This talk gives an overview of materials' aspect, charge carrier transport, and device physics of such diodes.

Furthermore, the use of solar photoenergy to reduce CO_2 into hydrocarbon based synthetic fuels is introduced. Such artificial photosynthesis type fuel production can simultaneously solve the energy storage and energy transport problems of photovoltaic electricity.

COMPUTATIONAL MATERIALS SCIENCE FOR ENERGY APPLICATIONS

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A key issue in the field of solar energy is the development of novel nanostructured functional materials for energy conversion and storage. In this context, computer simulations can contribute to rationalize and predict the physical and chemical properties of these materials. In this talk I will give a brief introduction to the computational methods with particular emphasis on density functional theory. I will show how this method and its extensions are currently employed to investigate diverse processes such as photoabsorbtion in dye-sensitized solar cells and the reversible formation of lithium oxides during discharge in lithium-air batteries. The simulations reproduce the experimental results and give insight into the role of different components of the systems under investigation.

MATERIALS FOR PHOTOVOLTAIC APPLICATIONS PREPARED BY PULSED LASER DEPOSITION

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