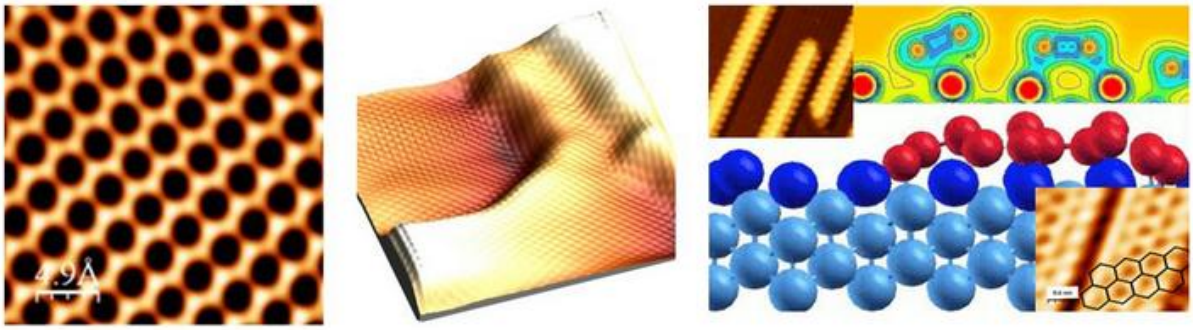
US-MOROCCO WORKSHOP ON NANO-MATERIALS AND RENEWABLE ENERGIES



Al Akhawayn University in Ifrane, Morocco

November 17 – 19, 2011

Organized by

US-National Science Foundation
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Euro-Mediterranean Conference on Materials and Renewable Energies
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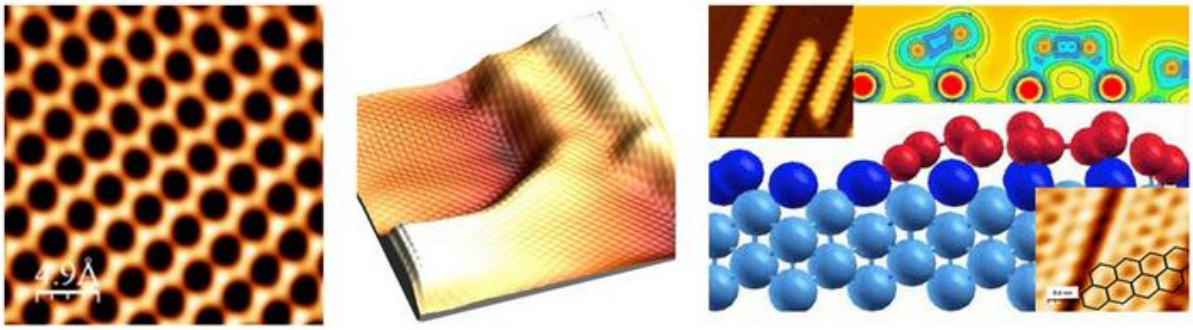

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School of Science and Engineering, Al Akhawayn University in Ifrane, Ave. Hassan II, B.P. 104, Morocco
http://emcmre-1.u-cergy.fr/workshop-fes.html

[1] *Travail publié avec le soutien du Ministère de l'Education Nationale, de l'Enseignement Supérieur, de la Formation des Cadres et de la Recherche Scientifique, sur les fonds gérés par le Centre National pour la Recherche Scientifique et Technique*

INTRODUCTION:

The US-Morocco international workshop on Nano-Materials and Renewable Energies is a platform for promoting scientific collaborations on nano-materials between researchers from the US and those from North Africa, in particular from Morocco. The workshop will also facilitate interaction between students from the US and from North Africa with researchers from Europe.

The workshop will include presentations from world experts on nano- materials in Europe, the US and North Africa. The focus will be on the potential use of these materials in renewable energies. These presentations will be delivered at an introductory level, and an overview of the recent advances on nano-materials, and their possible applications for renewable energies will be provided. Round table discussions between US scientists and those in Morocco will be held to explore possible collaborative projects. Special attention will be paid to materials for solar energy applications.

The workshop will bring unique experience for students and young scientists to build, and develop long-term relationships. The workshop will give opportunity for scientists to contribute to the quest for energy independence in Morocco as well as strengthening scientific research on nano-materials that have direct applications in renewable energies.

Organizing Committee:

M. Baitoul, University Sidi Mohamed Ben Abdellah, FSDM, Fes (Morocco)

H. Darhmaoui, Al Akhawayn University in Ifrane (Morocco)

A. Jorio University Sidi Mohamed Ben Abdellah, FSDM, Fes (Morocco)

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Mohammed Jamil Ouazzani, University Sidi Mohamed Ben Abdellah, FSDM, Fes (Morocco)

I. Zorkani, University Sidi Mohamed Ben Abdellah, FSDM, Fes (Morocco)

PROGRAM

Thursday, November 17

Check in and registration

Friday, November 18

08:00 - 08:30 **Registration - Board room in Building 1**

08:30 - 09:00 Opening remarks

Invited Presentations

09:00 - 09:45 Nanoscience: Connecting dots between Energy, Environment, and Ethics,
S. Ismat Shah, *Univ. of Delaware, USA*

09:45 - 10:30 Materials and devices design for highly efficient single and multi-junction organic solar cells
Qiquan Qiao, *South Dakota State University, USA*

10:30 - 11:00 **Coffee break**

11:00 -11:45 Characteristics of lithiatedtitania: concentration, morphology, pressure and nano effects
Handan Yildirim, *Argonne National Laboratory, USA*

11:45 - 12:30 Defect Energetics in prototype solar cell materials $CuInSe_2$
Ari P. Seitsonen, *Univ. of Zurich, Switzerland*

12:30 - 14:30 **Group Photo and Lunch - AUI restaurant**

14:30 - 15:15 Crystalline Silicon thin film solar cells: potential and challenges
Abdellilah Slaoui, *Institut d'Electronique du Solide et des Systèmes, Franc*

15:15 - 16:00 Boron nitride and graphene based honeycomb superstructures
Thomas Greber, *Univ. of Zurich, Switzerland*

16:00 - 16:30 **Coffee break**

16:30 - 17:15 Soft X-ray microscopy for advanced materials
Rachid Belkhou, *Syncrotron-SOLEIL, France*

17:15 - 18:00 Scanning probe microscopy for organic or hybrid photovoltaics
Philippe Dumas, *CINaM-CNRS, Marseille, France*

18:00 - 19:30 **Poster Session**

20:00 - 22:30 **GALA Dinner - AUI faculty club, AUI Annex**

Saturday, November 19

Invited Presentations

09:00 -09:45 Engineering optical properties of nanomaterials for solar cell applications
Talat S. Rahman, *Univ. of Central Florida, USA*

09:45 - 10:30 STMstudies of molecule adsorption on surfaces: is graphene the new nano-material?
Andrew Mayne, *Univ. of Paris Sud, France*

10:30 - 11:00 **Coffee break**

11:00 - 11:45 Experimental Solar Energy in Morocco
Adelkader Outzourhit, *Univ. Cadi Ayyad, Marrakech, Morocco*

11:45 - 12:30 Hybrid Inorganic-Organic Metal Phosphates and Phosphonates for Catalysis and Energy Applications
Abdessadek Lachgar, *Wake Forest University, USA*

12:30 - 14:30 **Lunch - AUI restaurant**

14:30 - 16:30 Round table discussion and closing remarks

16:30 - 17:00 **Coffee break**

Posters

VIBRATIONNAL AND THERMAL PROPERTIES OF FUNCTIONALIZED-MULTIWALL CARBON NANOTUBES- POLY (METHYL METHACRYLATE) NANOCOMPOSITE
B. Boussouari, M. Baitoul

IMPROVING THE PERFORMANCE OF PHOTOVOLTAIC STATIONS FOR PUMPING WATER AND LIGHTING INSTALLED IN THE DOUAR ZRAGTA OF THE RURAL COMMUNE OF ISLY PREFECTURE OF OUJDA ANGAD
E. Baghaz, M. F. Yaden, R. Gaamouche, K. Hirech, T. Mrabti, M. El Ouariachi, B. Tidhaf, F. Bagui, K. Kassmi

EFFECT OF OXYGEN PRESSURE ON THE OPTICAL AND STRUCTURAL PROPRIETIES OF RF SPUTTERED ZNO THIN FILMS.
L. Nkhali, M. Ait Ali, A. Outzourhit

POLARISABILITY OF A SHALLOW DONOR IN QUANTUM DOT-QUANTUM WELL
A. Lemnawar, A. Mmadi, K. Rahmani, I. Zorkani and A. Jorio

STUDIES OF $CD_{1-X}ZN_XTE$ THIN FILMS GROWN BY RF-SPUTTERING
Y. Elgabbas, H. Bellakhder, M. A. El Idrissi Raghni, A. Outzourhit

ELECTRONIC PROPERTIES OF SINGLE WALLED CARBON NANOTUBES / (POLY-3HEXYLTIOPHENE) COMPOSITES
M. Mansouri, A. Bakour, M. Baitoul, Jany Wéry

MAGNETIC PROPERTIES OF $Zn_{0.8}(Fe_{0.1},Co_{0.1})O$ DILUTED MAGNETIC SEMICONDUCTORS: EXPERIMENTAL AND THEORETICAL INVESTIGATION
O. MOUNKACHI, M. BOUJNAH, H. LABRIM, M. HAMDOUN, M. BELAICHE , A. BENYOUSSEF, A. EL KENZ, A. LAOULIDI, B. BELHOURMA, M. BHIHI.

MAGNETIC PROPERTIES OF $Zn_{0.9}(Mn_{0.05},Ni_{0.05})O$ NANOPARTICLE: EXPERIMENTAL AND THEORETICAL INVESTIGATION
O. MOUNKACHI, M. LAKHAL , H. LABRIM, M. HAMDOUN, M. BELAICHE , A. BENYOUSSEF, A. EL KENZ, A. LAOULIDI, B. BELHOURMA, M. BHIHI
.
STRUCTURAL, OPTICAL, AND ELECTRICAL STUDIES OF ZnMnO NANOCRYSTALS
O. Karzazi, A. Khodorov, K.C.Sekhar, S. Levichev, A. Chahboun and M. J. M. Gomes

CARBON NANOTUBES FOR EFFICIENT SMALL WIND TURBINES
Afrae Errarhout, H. Darhmaoui, K. Loudiyi, I. Zorkani

TiO_2-PALYGORKITE SUPPORTED PHOTOCATALYST NANOCOMPOSITES DEPOSITED BY CHEMICAL VAPOR INFILTRATION (CVI)
LAKBITA O., RHOUTA B., AMJOUD M , MAURY F., SENOCQ F., BOUNA L.

NUMERICAL MODELING OF THE THERMAL BEHAVIOR OF CORROSION ON REINFORCED CONCRETE
Naouar LAAIDI, Sougrati BELATTAR

QUANTUM DOTS AND INTERMEDIATE BAND SOLAR CELL
A. Mmadi, I. Zorkani, K. Rahmani and A. Jorio

SYNTHESIS AND CHARACTERIZATION OF FEW LAYERED GRAPHENE FOR RENEWABLE ENERGY APPLICATIONS
M. KHENFOUCH, M. BAÏTOUL M. MAAZA. O. BAJOU

ENERGY DYNAMICS IN NANOMATERIALS FOR QUANTUM DOT SOLAR CELLS
F. Xu , X. Ma , C. R. Haughn, J. Benavides, M. F. Doty and S. G. Cloutier

AN AB INITIO STUDY OF HYDROGENATION INDUCED METALLIZATION OF SIC001 (3X2)
James Westover, Abdelkader Kara

INVITED PRESENTATIONS

NANOSCIENCE: CONNECTING DOTS BETWEEN ENERGY, ENVIRONMENT, AND ETHICS

S. Ismat Shah

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Recent developments in nanoscience and technology have opened up new pathways for research related to energy and the environment. For energy related research, photovoltaics is arguably at the top of the list with the current focus on increasing efficiency of the devices made with Earth Abundant Materials (EAM) . The talk will survey current practices and problems with special emphasis on materials development, particularly nanomaterials. Solar energy can also be utilized in combination with a semiconductor to oxidize volatile organic compounds (VOC) either in air or in water. Semiconductors typically used for this purpose include TiO_2, WO_3, Fe_2O_3, ZnO, CdS, etc. Most of these materials have limitations that range from too high a band gap and therefore sensitizable only by the small UV portion of the solar spectrum (e.g. TiO_2) to lack of stability in aqueous medium (e.g. ZnO) to toxicity (e.g. CdS). TiO_2 is inter and stable but has a bandgap of 3.0 – 3.2 eV. The talk will review schemes to modify TiO_2 bandgap by either cation (V, Nd, etc. doping) or anion substitution (C, N, S, etc. doping) and the consequential effect of vacancies. Finally, the ethical issues related to the use of nanotechnology, particularly nanotechnology related to energy and environment will be discussed in order to evaluate the risks and benefits associated with this new technology.

MATERIALS AND DEVICES DESIGN FOR HIGHLY EFFICIENT SINGLE AND MULTIJUNCTION ORGANIC SOLAR CELLS

Qiquan Qiao

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Organic solar cells have the potential to spawn a new generation of light-weight, low-cost, and solar-powered products on thin and flexible substrates. However, the current energy conversion efficiency (8.4%) is still low for commercial applications. New materials and device designs are needed to increase the efficiency and make this technology available for large-scale applications. The major issues in organic solar cells include narrow spectral light harvesting and inefficient charge transport. To solve these issues, new conjugated polymers with optimized bandgaps and energy levels (highest occupied molecular orbitals, HOMO, and lowest unoccupied molecular orbitals, LUMO) need to be designed for significantly higher efficiencies in both single and multijunction organic solar cells. The dependence of cell efficiency on the polymer bandgaps and energy levels in organic solar cells will be presented, which will provide guidance for the engineering of new conjugated polymers. The interfacial layers between the subcells in the multijunction organic devices will also be discussed.

CHARACTERISTICS OF LITHIATED TITANIA: CONCENTRATION, MORPHOLOGY, PRESSURE AND NANO EFFECTS

Handan Yildirim, Jeff Greeley, and Subramanian Sankaranarayanan

Center for Nanoscale Materials Division
Argonne National Laboratory, 9700 South Cass Ave., Argonne, IL 60439
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Fast transport of ions in electrode materials is important for electrochemical performance, as fast insertion and de-insertion rates allow efficient cycling of ions in lithium ion battery anodes. Recently, efforts in this area have been devoted for the development of improved nanostructured electrodes, as they lead to reduced diffusion lengths and thus allow fast ionic transport. A fairly general understanding has been established regarding the effect of the nanoscale on the electrochemical efficiency of the electrodes. However, the atomistic details behind the enhanced performance, and the effect of morphology, are still not well understood, and such understanding is crucial for designing materials, which allow better electrochemical performance. This work probes such atomistic details to provide insights into the design of electrode materials with fast ion transport rates. Important factors such as mechanisms and energetics, together with the effects of dynamics, morphology and concentration are discussed for Li ion diffusion in bulk anatase, amorphous and rutile TiO_2. Additionally, such effects will be compared to those for the nanostructures. The structural transitions upon lithiation, and under pressure, will be discussed in detail.

The Li ion diffusion mechanism is found to depend on the morphology of the lattice. Our calculations show that diffusion of Li in anatase is 3D in nature, while that in rutile is 1D. The diffusion in rutile is found to be much faster than that in anatase and amorphous titania. Our simulations indicated that changing the Li ion concentration significantly modifies its diffusivity. However, the changes in diffusivities are found to differ from structure to structure, and are affected by the morphology of the lattice. Our results show that for both anatase and amorphous TiO_2, increasing the concentration increases diffusivities (up to 75% Li loading for anatase, and for all concentrations for amorphous), while the diffusivity decreases for rutile with increasing Li concentration. The reason for the decreasing diffusivity in the latter case is attributed to increasingly blocked diffusion sites, and increasing Li-Li repulsion. The effect of concentration on the diffusivity in amorphous is different than that for the crystalline structures, as the amorphous TiO_2 undergoes structural transitions that lower the barrier for diffusion.

We have identified a structural transition for lithiated amorphous TiO_2 when fully loaded. The new structure is a cubic phase, which provides faster Li diffusion. We find that the configurational energy and entropy of the cubic structure is lower than that of the amorphous titania. We have also examined the stability of the lithiated and the de-lithiated cubic structures by applying pressure at 300K, and find that the lithiated cubic phase is stable under a wide range of pressures, while de-lithiated cubic goes under phase transition to an amorphous. These results will be compared to those for the nanostructures.

ACKNOWLEDGMENTS

The computational facilities by CNM-ANL and Fusion Clusters are gratefully acknowledged. Use of the Center for Nanoscale Materials was supported by the U. S. Department of Energy, Office of Science, and Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357. The discussions are appreciated with the individuals at Nano-bio interface group at CNM, and C. Johnson at CSE.

The submitted manuscript has been created by UChicago Argonne, LLC, Operator of Argonne National Laboratory ("Argonne"). Argonne, a U.S. Department of Energy Office of Science laboratory, is operated under Contract No. DE-
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DEFECT ENERGETICS IN PROTOTYPE SOLAR CELL MATERIAL $CuInSe_2$

Laura Oikkonen[1], Maria G Ganchenkova[1], Ari P Seitsonen[2] and Risto Nieminen[1]

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There is a strong effort to find optimal materials for solar cells. A candidate is $Cu(In,Ga)Se_2$ (CIGS) that has a very high efficiency. There are several studies on this material, but still many of its basic material properties remain unexplained, like the atomistic structure of defects and their influence on the characteristics of CIGS [1].

We have performed electronic-structure calculations [2] using density functional theory to describe the CIGS material. In this contribution we concentrate on the material $CuInSe_2$ and in particular the intrinsic vacancies. This material has been used to produce photovoltaic modules [3]. We have used the HSE06 [4] screened, hybrid exchange-correlation functional that replaces 25 % of the GGA exchange by the Hartree-Fock exchange energy. This improves in particularly the description of the band gap.

Our results show that there are no ionization levels in the band gap of $CuInSe_2$ due to copper or indium vacancies, but the selenium vacancy has a deep acceptor level $\varepsilon(0/2-)$. The copper vacancy has a low formation energy, as generally believed from experiments.

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CRYSTALLINE SILICON THIN FILM SOLAR CELLS: POTENTIAL & CHALLENGES

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Crystalline silicon thin films, free standing or deposited on foreign substrates are considered as a very promising alternative approach to bulk silicon based cells. Cost reductions can be accomplished through the processing and the amount of silicon used. The carrier collection can be improved by light confinement provided by the highly reflective substrates or back contacts. Here the different methods used to form either free standing crystalline silicon films or thin silicon layers formed on foreign substrates by direct chemical vapor deposition (CVD) process or by metal, lamps or laser crystallisation of amorphous silicon will be reviewed. The structural and electronic quality of the silicon layers will be reported and potential and limiting factors towards high efficiency solar cells will be discussed.

On the other hand Silicon nanocrystals (Si-NCs) embedded in dielectric matrices as candidates to develop high efficient third generation SC based on silicon technology will be presented. This material has excellent properties such as its band gap energy can be tuned from 1.12 eV up to energies larger than 2 eV by controlling the size of the nanostructures, their crystalline state and/or their surrounding matrix. We will present the structural and optical characterization of single SiOxNy and multilayered system of SiO2/SiOxNy deposited by plasma-enhanced chemical-vapor deposition, varying the silicon rich oxynitride (SRON) layer thickness and composition. The potential of applying such nanostructures as photon shifters on conventional cells or as part of Si tandem cells is discussed.

BORON NITRIDE AND GRAPHENE BASED HONEYCOMB SUPERSTRUCTURES

Thomas Greber

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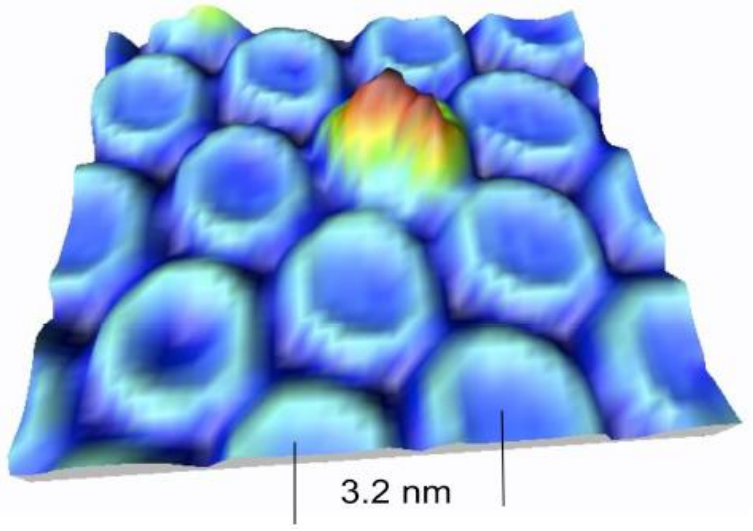
Single honeycomb layers of hexagonal boron nitride and graphene on Rh(111) and Ru(0001) form corrugated superstructures with about 3nm lattice constant. These structures are stable in air and may be used as templates for supramolecular architectures. The peculiar trapping mechanism for single molecules with a diameter of 1 to 2 nm is traced back to strong lateral electric fields within the nanostructure that can be measured with photoemission from adsorbed xenon [1].
Similarities and differences between hexagonal boron nitride and graphene will be highlighted [2].

Scanning tunneling microscopy image recorded at room temperature: One Cu-phthalocyanine molecule is trapped on the h-BN/Rh(111) nanomesh. The lattice constant of the superstructure is indicated from [3].



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SOFT X-RAY MICROSCOPY FOR ADVANCED MATERIALS

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The advent of ultra-bright synchrotron radiation sources has enabled the development and the renewal of X-ray microscopy methods. This open-up new route for studying advanced materials with spatial resolution in the 10nm range. As a matter of fact, the recent progress in the fabrication of nanostructures requires the development in parallel of new techniques capable to characterize theses new materials at a nanoscopic level. A technique which could study them combining good spatial (few nm) and time (submicrosecond) resolution and giving access to their structural and electronic properties, would be of primordial importance.

Soft X-ray microscopy is nowadays, a very good candidate for this purpose. It combines spectroscopy methods such as photoemission and absorption spectroscopies (giving access to the local structure, electronic, magnetic and chemical properties) with high spatial resolution (<10nm). Experimentally there are two different approaches. The first uses a well-focused photon beam which is scanned across the sample's surface. The second employs parallel imaging techniques making use of special electron optics. In this lecture, we shall review the principals of soft X-ray microscopy in synchrotron radiation emphasizing on their potential interest and application for studying nanostructures and advanced materials. A special attention will be dedicated to materials developed for solar and renewal energies.

SCANNING PROBE MICROSCOPIES FOR ORGANIC OR HYBRID PHOTOVOLTAIC

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[2] *Aix-Marseille Université. Contact : philippe.dumas@univmed.fr*

1) Context / Study motivation

The recent organic or hybrid photovoltaic (PV) stream made remarkable progress over the last years [1]. This stream is particularly interesting for two main reasons; 1) the low cost of the involved processes and 2) the possibility to use roll-to-roll technology allowing very large manufacturing flow [2]. However, in order to play a major role in the PV development, further progresses need to be made in durability on one hand and in conversion efficiency on the other hand. Indeed, a mass production of PV electricity will undoubtedly compete with other uses of the Earth resources such as, for example, the agriculture. Therefore, competitive conversion efficiencies for organic or hybrid PV components need to be achieved even though we are still far away from the Silicon technology [3]. In order to increase the efficiency, one will need to first improve the absorption of light of the existing PV cells. However, absorbing light is not the only improvement to be done, yet one also needs to recover the energy transferred to the exciton: that is to say to separate it and to efficiently recover the involved charges in the process. Unlike inorganic PV materials, the organic ones suffer from very poor electrical properties since the charges photo-generated cannot move over larges distances (typically few tens of nanometers) [4,5], facilitating charges recombination. Progresses could already be achieved only by addressing this issue.

Probing the matter with the relevant (nano) spatial scales is thus essential and inescapable. However, at these scales meaning well below the resolution limit of many optical microcopies, numerous existing characterization techniques are prohibited. One then needs to utilize more powerful microscopy techniques such as high resolution electronic microscopy or even better, local probe microscopies well-known for their efficiencies at the nanoscale. These latter gather various characterization techniques that we want to explore to deepen understandings on organic or hybrid PV mechanisms in order to significantly improve their performances. Atomic Forme Microscopy (AFM) is known to provide valuable structural information. We want to stress here Kelvin Probe Force Microscopy (KPFM) [6] under illumination. A brief description of the technique is given in Section 2, while the expected results and conclusions are summarized in Section 3.

2) Description of approach and techniques

As a response to the mentioned issues, we propose to correlate the macroscopic properties of a PV cell, measured with classical techniques (such as I/V curves under illumination), with its local properties measured by KPFM under illumination. The used organic PV cells are P3HT-PCBM blends and the hybrid PV cell is a mixture of PEDOT and Zinc Oxide (ZnO) particles. They are deposited on a conductive Indium Tin Oxide (ITO) substrate.

KPFM has been mainly developed over the last 10 years and is nowadays a powerful technique to access to the local surface potential. This surface potential may be measured via the capacitive force installed between the probe and the sample surface and linked to the charges accumulations. These charges originate mainly from the absorption of light in the PV layer. Since KPFM is implemented with no contact between the probe and the sample surface, local measurements are carried out at a zero current that are thus linked to the V_{OC} (Voltage Open Circuit) of the PV cell, see the scheme of the setup in Fig. 1. The resolution limitations here are mainly due to the radius of curvature of the probe and the working distance (probe-sample). Nevertheless, the achievable resolutions are compatible with the nanoscale morphologies of the mentioned PV samples. The local photo-electric response of the cells, at the relevant scales for charges transport, is therefore the ultimate objective. KPFM is indeed a powerful technique fully appropriate for this study. However, the best resolutions have been, for now, obtained with atomic force microscopy (AFM) working with very short working distances (non contact mode) under restrictive conditions of UHV [7-9]. In our setup, we will work at atmospheric pressure with more appropriate and adapted geometries and modes for PV samples. Moreover, our measurement system will be coupled to an optical microscope to ease the illumination control. In particular, under pulsed illumination, the time dependence of V_{OC} can be registered [10]. It is highly sensitive to the amount of recombination losses in the sample which should be understood and controlled to improve the overall efficiency.

3) Results / Conclusions / Perspectives

Our study will be conducted on organic or hybrid PV cells deposited on ITO substrate (serving as one of the electrical contact). The KPFM probe is taken to be the second electric contact.

Local photo-electric measurements on a PV cell will be presented and correlated to the macroscopic performances (i.e. I/V curves under standard solar AM 1.5 illumination). The achieved lateral resolution under the exposed experimental conditions (as already mentioned, our experiment is conduced at atmospheric pressure) will be discussed. A comparison with the typical dimensions of the entanglement, between the components constituting the PV cells, will be then given. The long-term objectives of this study, together with results from other complementary (more standard) studies, will permit to identify, at the nanoscale, defects. These defects are indeed behind causes of losses and are limiting the organic or hybrid PV cells efficiencies. The aim is thus to identify these defects in order to improve the fabrication processes and therefore to improve the organic or hybrid PV cells performances.

The authors would like to acknowledge J. Ackermann at the CINaM for providing the test samples used in this study.

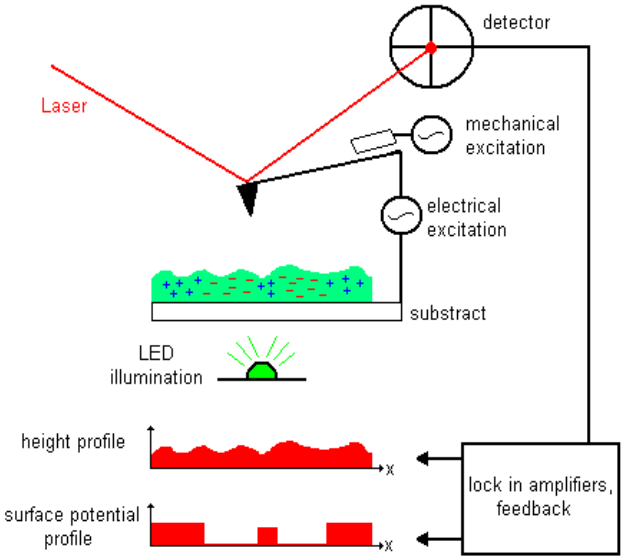

Figure 1: Scheme of the used KPFM setup under illumination.

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ENGINEERING OPTICAL PROPERTIES OF NANOMATERIALS FOR SOLAR CELL APPLICATIONS

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Plasmonic nanostructures are possible candidates for reducing the thickness of the photovoltaic absorber layers. Metallic nanoparticles, for example, could be tailored to couple and trap freely propagating plane waves from the Sun into an absorbing semiconductor thin film, or serve as sub-wavelength antennas in which the plasmonic near-field is coupled to the semiconductor. In each case, they are expected to enhance the efficiency of the solar cell. In this talk, after a brief review of the challenges and opportunities in the rational design of nanomaterials for solar cell application, I will present results of application of the time dependent density functional theory (TDDFT) approach to examine the optical properties of pure Au and Ag chains and those doped with transition metal atoms (Ni,Rh,Fe)[1]. Our results indicate that in the case of un-doped chains a collective plasmon mode is formed when the number of atoms is larger than ~ 10. The plasmon energy approaches asymptotically a value of ~0.6eV. In the case of chains with odd number of atoms, an additional low-energy excited state close to the plasmonic peak is found. This state comes from the unfilled bond between the even chain edge and the extra (odd) atom. In the presence of doping, the system acquires one or more local plasmonic excited states close in energy to the extended plasmon peak, which is especially pronounced in the case of Ni-doped chains. I will also discuss the role of the transition metal d-electron states in formation of the local plasmon modes. Additionally, I will present an example of manipulation of the optical properties of organic- and dye-molecule conjugated semiconductor nanoparticles to produce high efficiency visible photoluminescence, using the example of folic acid-conjugated titania and ceria nanoparticles.[2] Using DFT and TDDFT we find that the strong increase of the photoluminescence can be explained by electronic transitions between the titania surface oxygen vacancy states and the low-energy excited states of the FA/APTMS molecule anchored onto the surface oxygen bridge sites in close proximity to the oxygen vacancies.

Work supported in part by DOE Grant No. DOE-DE-FG02-07ER46354 and done in collaboration with V. Turkowski, N. Nayyar, D. Le, and A. Kabir.

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STM STUDIES OF MOLECULE ADSORPTION ON SURFACES: IS GRAPHENE THE NEW NANO-MATERIAL?

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Graphene is foreseen as a flexible, transparent and conducting substrate [1] that could efficiently replace Indium Tin Oxide (ITO) in Organic Light Emitting Diodes (OLED) [2] and organic photovoltaic devices [3]. To integrate graphene into these applications, an understanding of the electronic interactions between the molecules and graphene is crucial [4].

The Scanning Tunneling Microscope is the ideal technique for probing the electronic properties of these new nano-materials. Studies at the atomic-scale are vital if we are to improve the overall efficiency in hybrid organic-conducting devices. We will present STM observations on single layer graphene that allow us to pose a number of questions that are important for future devices.

1) We have used Scanning Tunneling Spectroscopy to probe the influence of atomic-scale point defects and step edges on the electronic properties of the clean graphene surface and the coupling to the underlying substrate (SiC).

2) We have looked at the adsorption of fluorescent organic molecules on SiC and graphene from a single molecule to a self-assembled layer of molecules [5]. These studies raise a number of crucial ideas that need to be considered; molecule-substrate interactions, intermolecular interactions, effects on the molecular states, the role of the surface states on electron transport. Both STS studies and STM manipulation experiments help us to probe what is going on.

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EXPERIMENTAL ASPECTS OF SOLAR ENERGY RESEARCH IN MOROCCO

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In this talk I will give a detailed account of the photovoltaic energy research at the Cadi Ayyad University since its creation in 1978. The materials, the device as well as the system aspects of our research efforts will be outlined. In particular, the recently installed PV-powered reverse osmosis desalination units and the PV-wind hybrid power plant will be descried. The hybrid renewable energy plant consists of 7.2kWp PV array coupled with a 5 kW wind turbine. It is used to provide green electricity to a small rural village in the province of Essaouira (Lkaria, Rural commune Sidi Ishaq). The power and energy management schemes of the hybrid plant will also be described. It's operational as well as performance parameters will be given as a function of time. The suitability of these systems for other villages will be discussed.

HYBRID INORGANIC-ORGANIC METAL PHOSPHATES AND PHOSPHONATES FOR CATALYSIS AND ENERGY APPLICATIONS.

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The early focus was in structural hybrid materials based on carbon-silicon networks, but recent efforts have focused on the design of functional hybrid materials that combine the chemical and physical activity of their components. Hybrid frameworks offer a wider range of structures and properties. For example, they can display selective heterogeneous catalysis and their electronic properties have attracted much interest.[i,ii] Research in this area is truly interdisciplinary and involves thorough knowledge of the two worlds of chemistry, organic and organic, each with significant contributions to the field of materials science. The main challenge is identifying the right combination of organic and inorganic molecular building blocks that enhances the properties of each component while reducing their limitations. This challenge provides a unique opportunity for synthetic chemists for developing new materials with synergetic behavior leading to improved performance or completely new properties.

The discovery of aluminophosphates (AlPOs) with zeolite-like structures and their potential applications in catalysis, ion-exchange and gas separation led to extensive research activity in the field of open-framework metal phosphates.[iii,iv] In recent years, significant progress has been made in the area of porous coordination solids formed of molecular building blocks connected by suitable multidentate organic ligands.[v] The combination of the robustness of inorganic frameworks with the versatility and chemical flexibility of organic ligands has led to a number of novel hybrid inorganicorganic open-framework materials, such as phosphonates, aminophosphates, aminoacides, and phosphatodicarboxylates.[vi] Here, we will describe the design, the synthesis and the structural and thermal stability characterization of some Indium and gallium hybrid phosphates and phosphonates recently prepared in our laboratory.

Figure 1 represents the structure of one of these phases recently prepared through hydrothermal synthesis.

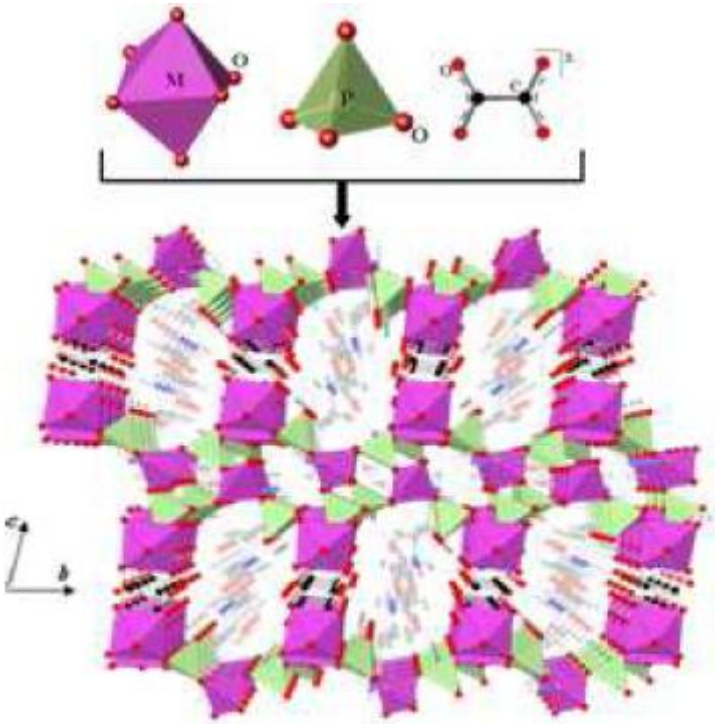

Figure 1. An example of what can be achieved by bringing together inorganic and organic components to form three-dimensional hybrid inorganic-organic open frameworks. In this case we combined gallium with phosphate groups and bridging oxalate ligands to form the compound shown.

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POSTERS

VIBRATIONNAL AND THERMAL PROPERTIES OF FUNCTIONALIZED-MULTIWALL CARBON NANOTUBES- POLY (METHYL METHACRYLATE) NANOCOMPOSITE

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The carbon nanotubes are most promising materials for the future of technology according to their exceptional electronic, electric, thermal …properties, in particular in terms of applications in nanometric devices. However, among unsolved problems with respect to applications of carbon nanotubes-polymer composites their dispersion at high concentrations. The purpose of the present work was to optimize the carbon nanotubes dispersion and elaborate composites material containing poly (methyl metacrylate) (PMMA) as matrix. The dispersion of the functionalized-MWCNTs in the polymer matrix was achieved using solvent. Properties of these nanocomposites, as well as the type of interactions between their components was obtained by using Environnemental Scanning Electron Microscopy (ESEM), Raman spectroscopy, Fourier transform infrared spectroscopy (FT-IR) and thermogravimetric analysis (TGA). The vibrational spectra of the PMMA confirmed the covalent interaction with the functionalized-MWCNT. The thermal analysis indicated an improvement of the thermal stability of the composite compared to the pristine PMMA.

Keywords:
Carbon nanotubes, nanocomposites, poly(methyl metacrylate), dispersion, thermogravimetric

IMPROVING THE PERFORMANCE OF PHOTOVOLTAIC STATIONS FOR PUMPING WATER AND LIGHTING INSTALLED IN THE DOUAR ZRAGTA OF THE RURAL COMMUNE OF ISLY PREFECTURE OF OUJDA ANGAD

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Today, the renewable energy of photovoltaic (PV) is the most realistic alternative that can address the issue of exhaustion of translational energy and environmental problem. The eastern region has enormous potential in solar energy; it receives an amount of energy of about 2500 kWh/m² per year. This is very favorable for the installation of photovoltaic stations of pumping and domestic lighting, and thus their improvements through the PV systems that are currently news.

In this context, we have installed in the United Nations program (PNUD) Art Gold Morocco two stations, lighting and pumping domestic for Douar Zragta in the rural municipality of the prefecture Isly Oujda Angad (Figure 1). The objective of this initiative is in the one hand contribute to the improvement of living conditions of the population of isolated sites, and in another hand promote PV systems realized in the laboratory . In this communication we present a description of these stations and the first results in terms of energy losses due to the absence of PV systems realized in the laboratory (MPPT control, tracking the sun, cruise charge / discharge , ...). The results obtained show that the energy losses can reach 30%. These lines induce loss of 33% of the cost of installation. Looking ahead, we aim to improve reliability and the two stations by reducing all energy losses (installation, adjustment, tracking the sun, charge control discharge / discharge ...) and the cost of facilities.

Keywords:
Photovoltaic System (PV), lighting and pumping domestic PV panels, Pspice simulator, loss of energy, sun tracker, solar controller, solar batteries.

Figure 1 : Photovoltaic stations for domestic lighting and pumping of

Acknowledgment

This work is supported by:

- programme Thématique d'Appui à la Recherche Scientifique (PROTARS III) D43/06,
- de la Coopération Marocco-Belge, CUI -2008-2012, « Commission Universitaire Institutionnelle de la CUD (Coopération Universitaire pour le développement), Energies renouvelables: Photovoltaïques.
- programme des Nations Unis au Développement PNUD Art Gold du Maroc, 2008 2 ENV OO.

EFFECT OF OXYGEN PRESSURE ON THE OPTICAL AND STRUCTURAL PROPRIETIES OF RF SPUTTERED ZNO THIN FILMS.

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Faculté des Sciences Semlalia-Marrakech

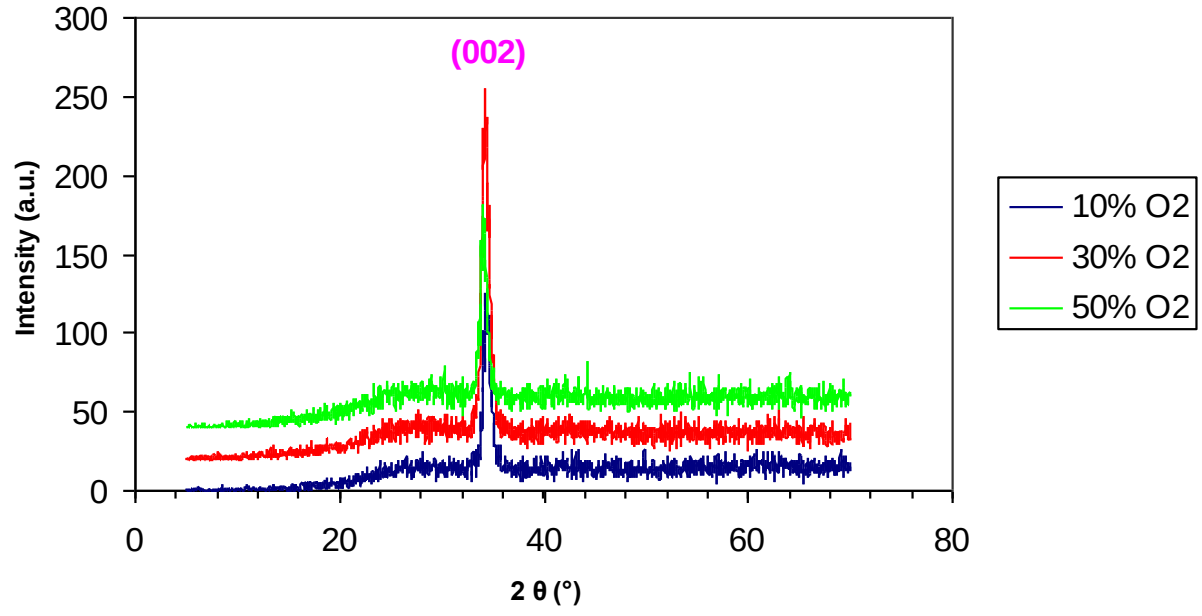
ZnO thin films were deposited by RF sputtering using a pure Zn target in an Argon-oxygen atmosphere with different Ar:O_2 gas mixtures. The following Ar:O_2 ratios of (9:1), (7:3) and (5:5) were studied.

Structural properties, of the as-deposited thin films, investigated by X ray Diffraction (XRD) technique. Optical properties (especially the refractive index, absorption coefficient and optical band gap) were measured by optical transmission measurements in the Ultraviolet-Visible-Near Infrared (UV-Vis-NIR) wavelength range.

The XRD diagrams show that the deposited ZnO thin films are polycrystalline in nature with the size of crystallites varying with O_2 gas.

The optical band gap energy of the produced ZnO thin films changed with O_2 gas contents, namely as the O_2 content in the sputtering gas is increased, the band gap energy and infrared-extrapolated refractive index decreased.

Fig.3 X-ray spectra of ZnO thin film as a function of oxygen percentage in the gas mixture



POLARISABILITY OF A SHALLOW DONOR IN QUANTUM DOT-QUANTUM WELL

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Using a variational method in the effective mass approximation, we have calculated the binding energy and the polarizability of shallow donor impurities in spherical Quantum Dot – Quantum Well under an applied electric field. We have considered an infinite confinement model to describe the barriers on the dot boundaries. We present our results as function of the size of the dot and several values of the electric field strength. The binding energy is found to strongly depend on the inner and the outer radius of the QDQW, also it depends strongly on the donor position.

STUDIES OF $CD_{1-X}ZN_XTE$ THIN FILMS GROWN BY RF-SPUTTERING

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The rf-sputtering method was used to prepare $Cd_{1-x}Zn_xTe$ thin films of different compositions on glass substrates. The films were subsequently annealed at 300 °c for 2 hours. SEM observations have been used to investigate the surface morphology of the films. XRD characterizations confirm the formation of ternary with preferential (111) orientation (Figure. 1).The UV-Vis-IR measurements of the films show that exhibit a high transmission (80%) and the gap of the film was found to be around 1.6 eV (Figure. 2).

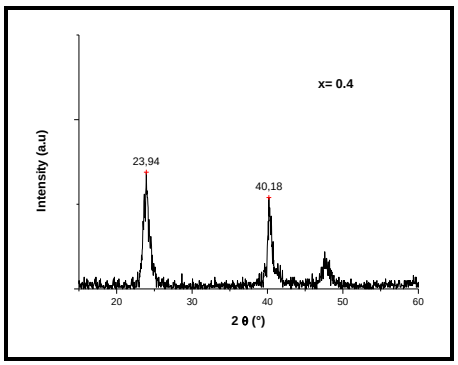

Fig. 1. XRD patterns of annealed sample at 300 °C.

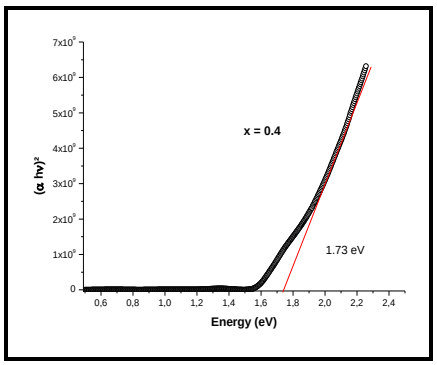

Fig. 2. Variation of $(\alpha h\upsilon)^2$ as a function of the energy $h\upsilon$

ELECTRONIC PROPERTIES OF SINGLE WALLED CARBON NANOTUBES / (POLY-3HEXYLTIOPHENE) COMPOSITES

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Organic solar cells, electronic and optoelectronic devices based on organic semiconductors have attracted much attention in the last few years. Using organic materials as active materials in these devices is due to the low-cost processing, mechanical flexibility, light weight and color-tunability. Among these materials, Poly (3-hexylthiophene) (P3HT) and carbon nanotubes are promising candidates for organic photovoltaic owing to their exceptional physical properties.

This work report on the effects of single walled carbon nanotubes Hipco (SWNT) dispersion in the conjugated soluble polymer poly (3-hexylthiophene) P3HT on the electronic properties of this composite. UV-visible absorption, Raman scattering showed that the insertion of SWCNT into the polymeric matrix (P3HT) led to a high order in both the P3HT and carbon nanotubes. In addition, we show that the quenching of the photoluminescence of the P3HT was achieved for the concentration of carbon nanotubes of 1W%.

Keywords: Poly(3-hexylthiophene), Single-wall carbon nanotube, nacomposite , Raman scattering, UV-Vis, photoluminescence

MAGNETIC PROPERTIES OF $Zn_{0.8}(Fe_{0.1},Co_{0.1})O$ DILUTED MAGNETIC SEMICONDUCTORS: EXPERIMENTAL AND THEORETICAL INVESTIGATION

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Structural and magnetic properties of $Zn_{0.8}(Fe_{0.1},Co_{0.1})O$ bulk diluted magnetic semiconductor have been investigated, using X-ray diffraction (XRD) and magnetization measurements. This sample has been synthesized by co precipitation route. Study of magnetization hysteresis loop measurements infer that the bulk sample of $Zn_{0.8}(Fe_{0.1},Co_{0.1})O$ shows a well-defined hysteresis loop at Tc (200K) temperature, which reflects its ferromagnetic behavior. Hydrogenation treatment was used for the control of phase separation. Based on first-principles spin-density functional calculations, using the Korringa-Kohn-Rostoker method (KKR) combined with the coherent potential approximation (CPA). The Ferromagnetic states energy was calculated and compared with the local-moment-disordered (LMD) state energy. Mechanism of hybridization and interaction between magnetic ions in $Zn_{0.8}(Fe_{0.1},Co_{0.1})O$ is also investigated.

Keywords: Diluted magnetic semiconductors,Ferromagnetic, hydrogen treatment, Ab-initio calculation, ZnO, Spintronic.

MAGNETIC PROPERTIES OF $Zn_{0.9}(Mn_{0.05,}Ni_{0.05})O$ NANOPARTICLE: EXPERIMENTAL AND THEORETICAL INVESTIGATION

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We report the synthesis of nominal 5% of Mn and Ni co-doped nanocrystalline particles by co-precipitation method. X-Ray diffraction data revealed that $Zn_{0.9}Mn_{0.05,}Ni_{0.05}O$ crystallizes in the monophasic wurtzite structure. DC magnetization measurement showed that the simple are paramagnetic at room temperature. However a large increase in the magnetization is observed below 50K. This behavior, along with the negative value of the Wiess constant obtained from the linear fit to the susceptibility data below room temperature, indicate ferromagnetic behavior. The origin of ferromagnetic is likely to be either the intrinsic characteristics of the sample, confirmed by energy stability calculated from ab-initio calculation.

Keywords: Diluted magnetic semiconductor, ZnO, co-precipitation synthesis Ab-initio calculation.

STRUCTURAL, OPTICAL, AND ELECTRICAL STUDIES OF ZnMnO NANOCRYSTALS

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The increasing energy demand in the near future will force us to seek environmentally clean alternative energy resources. The emergence of nanomaterials as the new building blocks to construct light energy harvesting assemblies has opened up new ways to utilize renewable energy sources [1]. Nanostructured Mn doped zinc oxide (ZnMnO), has attracted much research interest because of its potential applications for high-performance optoelectronic devices such as light emitting diodes and photovoltaic cells [2].

In this work, ZnMnO nanocrystals were grown by pulsed laser deposition [3]. Different growth and annealing conditions were achieved. The structural properties of thin films were characterized by Grazing Incidence X-rays diffraction and Grazing Incidence Small Angle Scattering techniques. The optical properties were studied by absorption technique. Hall Effect technique was used to estimate the conductivity and free carriers. We have been able to correlate the nanocrystals conductivity and the free carrier's concentration with the amount of defect in the studied films.

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CARBON NANOTUBES FOR EFFICIENT SMALL WIND TURBINES

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The low energy efficiency of small wind turbines has been one of the main barriers to widen utilization of this kind of turbines in distributed power production. This is why windmill technology companies have addressed this challenge by developing an awarded solution that utilizes nanotechnology in its blades. Carbon nanotubes make the blades stronger and lighter and improve energy efficiency.
This technology uses in wind turbine blades carbon nanotubes and epoxy that binds the nanotubes. As a result, the blades are approximately 50% lighter than the contending glassfiber blades. The blades are also stronger, due to the fact that carbon nanotubes are 100 times stronger than steel.

The strength and the low weight provided by the use of carbon nanotubes filled epoxy allow longer windmill blades to be used, thus increasing the amount of electricity generated by each windmill.

TiO_2-PALYGORKITE SUPPORTED PHOTOCATALYST NANOCOMPOSITES DEPOSITED BY CHEMICAL VAPOR INFILTRATION (CVI)

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Palygorskite fibrous clay mineral, isolated from natural Moroccan clay picked up from Marrakech High Atlas was used for preparing TiO_2 supported photocatalysts, by a dry OMCVD (organometallic chemical vapor deposition) process with titanium isopropoxide as precursor. Along the vertical reactor, the starting clay material was placed at three different positions: the top (inlet) (sample P-1), the middle (Pal-2) and the bottom (outlet) (Pal-3). The different functionnalized materials were characterised using X ray diffraction (XRD), scanning electron microscopy (SEM) equipped with analysis system (EDS), infrared spectroscopy and their photocatalytic activity was evaluated under UV radiation against the degradation of a model pollutant, namely the Orange G (OG). The characterization results showed that TiO2 anatase was successfully deposited on fibrous palygorskite for all the clayey samples. Nevertheless, the distribution mode as well as the coverage area of anatase particles on palygorskite fibers depends on the position of the starting clay mineral in the reactor. Indeed, the most homogeneous distribution and the most extended coverage area were obtained for the sample placed at the top (sample Pal-1), followed by that placed at the middle (Pal-2) and finally that placed at the bottom (Pal-3). Correlatively, the photocatalytic activities exhibited by the different samples (Figure 1) increased according to the following order: Pal-1 > Pal-2 > Pal-3.

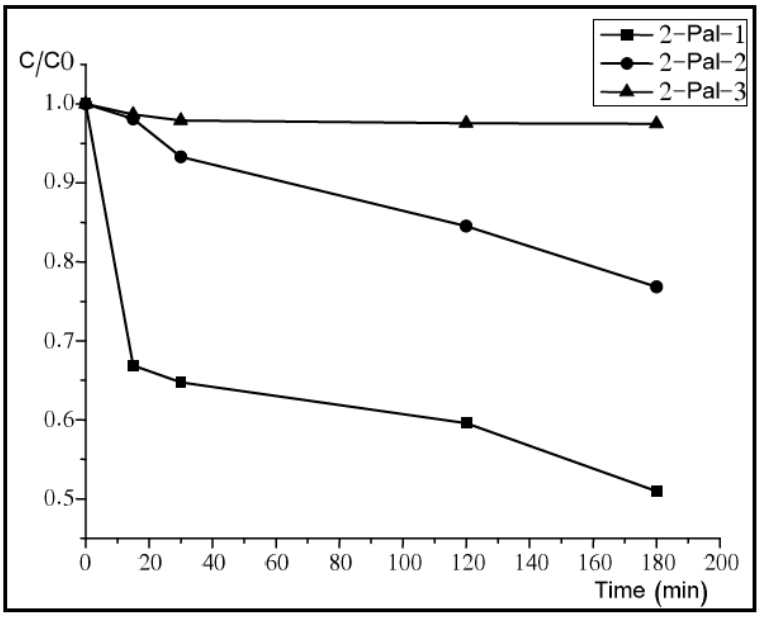

Figure 1: Variation of OG concentration versus UV irradiation time and sample position in the reactor after heat-treatement at 450° C for 4 hours.

These preliminary results are promising and demonstrate the possibility to functionalize natural Moroccan clay minerals powders by depositing nanosized particles of photoactive TiO_2 anatase by mean of dry OMCVD process. Likewise, this study reveals that the elaboration conditions need to be further optimized to prepare efficient supported photocatalysts. All these results will be presented and discussed in details.

NUMERICAL MODELING OF THE THERMAL BEHAVIOR OF CORROSION ON REINFORCED CONCRETE

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The bars in the concrete require a regular and permanent control in order to avoid the risks caused by the corrosion. In this work we present a thermal method of non-destructive testing of the structures, based on numerical modeling in three dimensions. The goal is to study the detectability and the behavior of rust in the steel in transient mode by using a thermal characterization, to present a limiting corrosion rate value which this technique is not reliable. The model of a parallelepipedic structure of concrete containing armatures of cylindrical form is adopted. This structure is supposed to be excited in the higher face by a heat flux, the lower face being maintained at constant temperature and the others faces are supposed thermically isolated.

Keywords: Corrosion rate, Infrared thermography, Reinforced concrete.

QUANTUM DOTS AND INTERMEDIATE BAND SOLAR CELL

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The effect of quantum dot implementation in intermediate band solar cell is presented in this poster. An intermediate band solar cell contains three bands: a conduction band, a valence band; and an intermediate band. The addition of an intermediate band augments the photogeneration of carriers. These additional carriers allow for an increased theoretical efficiency as compared to a conventional homojunction solar cell. The latter is necessary to ensure both a supply of electrons capable of photon induced transition to the conduction band as well as a large population of holes that allow photon induced electrons to transition from the valence band to the intermediate band. This novel material system is selected based upon a refined set of design rules that include a requirement that the quantum dot/barrier pair offer a negligible valence band. With such a design rule the existence of hole levels is avoided, thus reducing band gap narrowing at the valence band edge and the existence of mini bands below the intermediate band.

The intermediate band with respect to the conduction band is approximated by the ground state energy of a single electron in a single quantum dot heterojunction. The ground state energy is calculated with the radial Schrodinger equation with a Hamiltonian whose potential is composed from the step-like conduction band of the quantum dot heterojunction and the 1/r electrostatic potential of the hydrogenic impurity. The position of the intermediate band is tuned by adjusting the radius of the quantum dots. By assuming that the centrally located impurities are ionized, the location of the Fermi energy is guaranteed to be within the intermediate band.

SYNTHESIS AND CHARACTERIZATION OF FEW LAYERED GRAPHENE FOR RENEWABLE ENERGY APPLICATIONS

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Graphene proves strongly its particularity like nanomaterial which combines many important properties. The recent emergence of this stable two-dimensional (2-D) carbon has initiated a rapid exploration of its potential in a broad range of fields such as solar cells, nanoelectronics, sensors, catalysis and nanocomposites.
In the field of renewable energy, a critical aspect of any OPV photo-electronic device is a transparent conductive electrode, graphene, a highly conductive and highly transparent, has high potential to fill this role. The amount of electrical charge stored per weight of this material has already rivalled the values available in existing ultra capacitors, and modelling suggests the possibility of doubling the capacity in the future. A sheet of graphene was able to generate 100 nanowatts of power via Hydroelectricity process, which should be enough to power tiny sensors.
The main goal of this work is the mass production of good quality few layered graphene sheets. The quality of our product was investigated using structural and morphological characterization techniques.

Keywords: graphene, nanopowder, renewable energy

ENERGY DYNAMICS IN NANOMATERIALS FOR QUANTUM DOT SOLAR CELLS

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The dynamics of energy transfer in nanostructured materials are of critical importance for the development of new materials for photovoltaic energy conversion. Time-resolved photoluminescence (TRPL) is a powerful tool for characterizing energy transfer and nonradiative relaxation processes that occur on ultrafast time scales. We use TRPL to study charge transfer and recombination mechanisms in nanocrystalline thin films created by crosslinking colloidal quantum dots with benzenedithiol (BDT) and ethanedithiol (EDT) ligand-exchange treatments. The TRPL data allows us to identify an exciton funnelling process that "recycles" excitons bound to surface states. Our results confirm that energy transfer depends strongly on quantum dot proximity and cross-linking treatment. The results suggest approaches for engineering thin film structures with enhanced energy transfer and device efficiencies.

AN AB INITIO STUDY OF HYDROGENATION INDUCED METALLIZATION OF SIC001 (3X2)

James Westover, Abdelkader Kara

University of Central Florida

We will present results for the band structure of hydrogenated Silicone Carbide (001) (3x2) surface with various levels of hydrogenation. These band structures were obtained using density functional theory with a generalized gradient exchange correlation function. Further, the calculations reveal the following scenario.
Initially, Hydrogen atoms saturate all the dangling bonds of the surface dimers. This in turns allows for the subsequent H atoms to bind with Si atoms in the second layer. Those new bonds for the appropriately hydrogenated surface cause a “metallization" of the surface. Hydrogenation beyond that brings the system to its semiconducting state.

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