

**STRONG KINETIC ISOTOPE EFFECT IN THE DISSOCIATIVE  
CHEMISORPTION OF H<sub>2</sub> ON A PdO(101) THIN FILM**

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In the present study, we investigated the dissociative chemisorption and oxidation of H<sub>2</sub> on a PdO(101) surface under ultra high vacuum conditions by means of temperature programmed desorption (TPD) and temperature programmed reaction spectroscopy (TPRS). We find that H<sub>2</sub> chemisorbs into a molecular state on PdO(101) and that this state acts as a precursor to H<sub>2</sub> dissociation at low temperature. The dissociated products react with the PdO surface during continued heating, producing H<sub>2</sub>O which desorbs near 350 K. Similar experiments using D<sub>2</sub> support the conclusion that a molecularly adsorbed dihydrogen species mediates the initial dissociation, and reveal a strong kinetic isotope effect (KIE) for this reaction. Specifically, nearly all of the H<sub>2</sub> adsorbed at 75 K undergoes dissociation, whereas a much smaller fraction of adsorbed D<sub>2</sub> dissociates. Evaluation of DFT calculations leads us to conclude that quantum mechanical tunneling gives rise to the strong KIE. This study provides insights for understanding the pathways of hydrogen activation and oxidation on PdO surfaces.

**NUCLEATION AND GROWTH OF OXIDE NANOWIRES SEEDED  
BY THERMALLY-STABLE SELF-ASSEMBLED MICELLAR Pt  
NANOPARTICLES**

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Two technologically important aspects for the applications of metal nanoparticles in the fields of catalysis, molecular electronics and plasmonics are discussed here: (i) the influence of the nanoparticle synthesis method and support morphology on thermally-driven coarsening phenomena, (ii) the high-temperature growth of oxide nanowires with tunable width, orientation, and spacing seeded by metal nanoparticles. Along those lines, a comparison between evaporated Pt nanoparticles supported on pristine TiO<sub>2</sub>(110) and on polymermodified TiO<sub>2</sub>(110) and micelle-based Pt nanoparticles is established. Furthermore, on self-assembled micellar Pt and Au/TiO<sub>2</sub>(110) samples, the growth of TiO<sub>2</sub> nanowires at high temperature is shown.

Keywords: Pt, TiO<sub>2</sub>(110), micelle, nanoparticle, nanowire, coarsening, STM

## INFRARED SURFACE PLASMON RESONANCES ON NOBLE METAL, SEMIMETAL, AND SEMICONDUCTOR GRATINGS

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We report the excitation of surface plasmons on lithographically produced lamellar gratings of different amplitude formed from the noble metal Ag, the semi-metals Sb, Bi, and graphite, and the semiconductors Si and CuSnS. The IR sources used were quantum cascade and CO<sub>2</sub> lasers at wavelengths 6.1, 9.25, and 10.59 microns. The resonance absorption of radiation at the appropriate angle of incidence is compared with calculations using experimental permittivity values. Results allow determination of an empirical wavelength and grating-amplitude dependent surface impedance modulation parameter, which may be used in the design and optimization of surface plasmon grating couplers.

## STM INVESTIGATION OF PdO(101) THERMAL DECOMPOSITION

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The oxidation of transition metal surfaces involves the development of a variety of oxygen states which can have distinct properties. In particular, different surface oxygen states can have unique reactive properties, which could dramatically alter the catalytic behavior of a transition metal surface. Preparing well ordered oxygen states can provide further insights into these properties. In this study we used scanning tunneling microscopy (STM) to investigate the structure of bulk like PdO(101) grown on a Pd(111) surface under ultrahigh vacuum (UHV) conditions. We also investigated the structural changes caused by annealing and partially decomposing the PdO(101) thin film in vacuum. We observe that PdO(101) grows in a patch like network that is well distributed across the surface. Upon annealing the PdO(101) surface, the patch like network is replaced by large well ordered islands. We also observe several types of oxygen domains during decomposition of the PdO(101) thin film, which gives insight into the atomic-level mechanisms governing oxide reduction. These results demonstrate the ability to grow a well ordered thin film which can provide a platform for understanding the role that oxidation plays in modifying the reactivity of Pd surfaces under practical reaction conditions.

## GOLD-BLACK AS IR ABSORBER AND SOLAR CELL ENHANCER

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Infrared absorbance and visible/near-IR excited plasmon resonances are investigated in gold-black, a porous nano-structured conducting film. Polymer infusion (for hardening) generally reduced absorbance in the long wave IR but has little effect at THz wavelengths. The characteristic length scales of the structured films vary considerably as a function of deposition parameters, but the absorbance is found to be only weakly correlated with these distributions. Initial investigations of gold-black by photoelectron emission microscopy (PEEM) reveal plasmon resonances, which have potential to enhance the efficiency of thin film solar cells. For films with different characteristic length scales, the plasmon resonances appear in structures with similar length scales.

## REMOTE PLASMA ASSISTED ATOMIC LAYER DEPOSITION OF HfN<sub>x</sub>C<sub>y</sub> THIN FILMS

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As a transition metal nitride with superior physical and chemical properties, hafnium nitride (HfN) has attracted a lot of interest in recent years. Its high melting point (3380°C) high hardness, thermal stability, chemical inertness, low bulk resistivity (33 μΩ cm), and low work function make thin films of hafnium nitride useful as protective coatings on high speed cutting tools, as a gate electrode and diffusion barrier material in integrated circuit (IC) devices and as a cold cathode material in field emission applications. Different technologies for preparing hafnium nitride thin films have been investigated, including reactive sputtering, direct sputtering of a compound target, ion implantation, chemical vapor deposition (CVD) and atomic layer deposition (ALD). Among these technologies, sputtering is a proven method for achieving high quality and stoichiometric thin films. However, the less explored CVD and ALD methods are attractive as they can result in more smooth and conformal thin films, which is quite important for the application of IC devices. Our research is focused on the ALD process of hafnium nitride thin film deposition. Tetrakis (dimethyl amido) hafnium (IV) (TDMAH) and a hydrogen plasma were used as the metallorganic precursor and reducing agent respectively to deposit HfN thin films on Si(100) and oxidized silicon substrates. A remote, inductively coupled plasma was used to minimize the effect of ion bombardment during film deposition. A LabVIEW program enabled control of the plasma assisted ALD process, so that the plasma was generated during the hydrogen cycle only. Stoichiometry of the as-deposited thin films was studied by X-ray photoelectron spectroscopy (XPS). A depth profile analysis showed a different chemical composition on the top surface (2~3nm) from that of the bulk while carbon was incorporated in the bulk thin film in the form of hafnium carbide (10~20%). Atomic force microscopy (AFM) measurements show the topography of the as-deposited thin film is quite smooth with a RMS roughness under 1nm. X-ray diffractometry (XRD) hasn't shown any crystalline features under our experimental conditions, probably due to incorporation of carbon, while the resistivity of as-deposited thin films measured by a four point probe is between 104~105 μΩ cm indicating a post deposition treatment or more optimization of the deposition condition is needed before the films can be used as a metallic layer for ICs. Optimization of the plasma chemistry by using inert He gas will be explored as well as the effect of a forming gas anneal.

**CHARACTERIZE THE CHROMATIN DYNAMICS  
BY HIGH RESOLUTION MULTIPLE NUCLEAR BODY TRACKING**

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Cell nucleus plays the most important role in cell functioning including gene expression and post transcriptional regulation. It remains the open question to the physical role of real-time architecture of chromatin and its mediation with gene regulation. In this work, we developed the multiple-particle tracking method based on the Kalman filter to study the dynamics of green fluorescence labeled NAC-1 nuclear bodies with both high temporal and spatial resolution. NAC-1 nuclear bodies are located in the interchromatin area and fluorescence recovery after bleaching analysis shows NAC-1 nuclear body has approximately 50% of immobile fraction. Mean square displacements (MSD) of nuclear bodies' movement show that nuclear bodies undergo the sub-diffusive behavior in the nucleus. The mobility of nuclear bodies is negatively related to its size and chromatin structural change by ATP depletion or inhibition of transcription also affected the MSD of NAC-1 nuclear bodies. Chromatin condensation increases the mobility of NAC-1 but stabilizing the chromatin structure greatly decreases the NAC-1 mobility. To conclude, the mobility of NAC-1 is highly associated with the chromatin dynamic structure.

## 2-PROPANOL OXIDATION OVER SUPPORTED Pt NANOPARTICLES: A STUDY OF CATALYTIC PERFORMANCE AND PARTICLE MORPHOLOGY

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The catalytic oxidation of alcohols is of great interest in industrial applications where partial oxidation may be required in chemical synthesis processes while complete oxidation can be used as a pollution control method. This study discusses structure-reactivity relationships in the oxidation of 2-propanol by Pt nanoparticles supported on  $\text{Al}_2\text{O}_3$  and  $\text{ZrO}_2$ . Size-selected nanoclusters synthesized via inverse micelle encapsulation are characterized by atomic force (AFM) and transmission electron microscopy (TEM) as well as X-ray photoelectron spectroscopy (XPS), and extended X-ray absorption fine structure spectroscopy (EXAFS). The performance of our Pt nanoparticle samples is evaluated in terms of catalytic activity (conversion) and selectivity in a packed-bed mass-flow reactor.

## LUMINESCENCE AND STRUCTURE CHARACTERIZATION OF SELF-ACTIVATED BISMUTH GERMINATE SCINTILLATION NANOCRYSTALS

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To date, scintillation crystals have been made with complex single crystal growth methods such as Czochralski and Bridgeman methods, which frequently result in high costs and limited crystal size. Therefore, development of low-cost processes for larger area scintillation materials is imperative. In this study, a facile sol-gel method was used to prepare self-activated bismuth germinate (BGO) nanocomposites for scintillation detection use. Flower- and coral-like BGO crystals were synthesized and their photoluminescent and structural properties were studied. XRD data showed good crystallinity without any impurity phase of as-prepared and calcined samples for coral-like BGO, while flower-like BGO exhibited a second phase of BGO after being calcined at 500 C for 2 h in air. Both flower- and coral-like BGO crystals exhibited broad emission from 350 to 700 nm assigned to  $\text{Bi}^{3+}$  transitions from  $^3\text{P}_{0,1,2}$  and  $^1\text{P}_1$  to  $^1\text{S}_0$  with the peak located at 480 nm. The thin film quantum yield (QY) was determined via an integrating sphere. Coral-like BGO calcined at 600 C for 2 h showed QYs up to ~80% when excited at 280 nm. Moreover, a novel  $\text{Bi}_2\text{O}_3/\text{BGO}$  core/shell scintillating composite was synthesized. The time-dependent morphology and structure evolution were studied to determine the formation mechanism. The scintillation response under irradiation and potential for the application of these materials in scintillation detectors will also be discussed.

## PREPARATION OF HIGH ENERGY STEP EDGES ON TiO<sub>2</sub>(110) BY GRAZING INCIDENCE ION SPUTTERING

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Step edges on metal oxide surfaces are important sites for adsorption and reactions of molecules. Their investigations by surface science methods require a reliable approach for their synthesis. Unfortunately, only step edges with low formation energies can be readily prepared by formation of vicinal surfaces. Often minority sites that are thermodynamically unstable are, however, the more reactive sites. The inherent instability of such step edges make it challenging to prepare them with a high density at single crystal surfaces for their characterization. Here we present a new method that can achieve the preparation of metastable step edges<sup>1</sup>. This method utilizes a kinetic approach to align step edges along a predefined direction and thus is capable of creating surfaces with a high density of metastable steps. A low energy Ar<sup>+</sup> ion beam is directed at a surface at a grazing incidence angle causing preferential sputtering of step edges oriented normal to the ion beam azimuth. We have investigated this mechanism extensively and present the characterization of the surface evolution with sputter times and extract information about the enhancement of the sputter yield at step edges. As consequence of preferential step edge sputtering, an alignment of steps parallel to the ion beam is achieved for prolonged sputtering. Furthermore, we have demonstrated that by directing the ion beam along specific crystallographic directions, certain step edge orientations can be stabilized even if they are thermodynamically unfavorable. Annealing causes these step edges to form more stable orientations. A combination of atomic resolution scanning tunneling microscopy and density functional theory allowed us to determine the atomic structure of these high energy step edges. We show that these step edges reconstruct to lower their energy similar to surface reconstructions. These results are a first step for understanding the properties of high energy step edges.

<sup>1</sup> T.Luttrell, W. Li, X. Gong, and M. Batzill, Phys. Rev. Lett. 102, 166103 (2009).

## **SUPRAMOLECULAR STRUCTURE OF POLY (3-HEXYLTHIOPHENE) ON GRAPHENE NANOSHEETS WITH IMPROVED COMPATIBILITY**

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Graphene, the single atom thick form of elemental carbon, has been the focus of intense research since it has emerged as an inexpensive substitute of carbon nanotube; but its limited availability enforced scientists to find its alternative and a new material -reduced graphene oxide (RGO) emerged, which shared many of the properties of the original graphene. Single layered RGO sheets are derived by chemical reduction of graphene oxide (GO) generated from the oxidation of pristine graphite by Hummer's method. The robust mechanical properties and semiconducting behavior of RGO nanosheets and its composites were explored for nanoelectronics and thus produced greater hope to make a revolutionary move from scientific research to exciting practical application. The aim of the current research is to promote RGO and its composites as a viable material in the field of nanoelectronics for the coming decade.

Single layer of graphite or "graphene" and poly(3-hexylthiophene)(P3HT) have received significant attention in fabricating organic electronics due to their superior charge mobility. Integrating P3HT and graphene nanosheets in a single composite material will open new prospects in aligning and forming molecular devices. Here, we report the self-assembled supramolecular P3HT structures on reduced graphene oxide (RGO) nanosheets with a possibility of achieving tunable electrical performance. Poly(3-hexylthiophene)(P3HT) supramolecular structures were fabricated on RGO through a bottom-up graphene induced crystallization process. The crystallization process monitored by in-situ UV-Vis spectroscopy clearly indicated that graphene could greatly enhance the P3HT crystallization. RGO has ordered pristine graphene structures separated by disordered domains. The P3HT nanowires formed on the graphene surface could connect the ordered "graphene-domains" of many individual sheets, forming bridges to bypass the insulating disordered domains. Such supramolecular structures will have potential applications in organic electronics such as thin film transistors and organic photovoltaic.

## COMPREHENSIVE HEMT RELIABILITY TESTING

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HEMT reliability testing not only determines device lifetime but identifies weaknesses and failure mechanisms. New and creative testing may be necessary to determine the reliability of new materials and structures. An in-house reliability test system provides the necessary flexibility to determine the best way of testing HEMT devices. Using commercial off-the-shelf power supplies and data acquisition equipment, we are designing a unique and flexible control system that will allow for many different tests: DC and RF, temperature, step/stress/recovery, high-speed pulse, and optical pumping, as well as combinations and automated sequencing of these tests to provide a comprehensive investigation. The initial station will provide for the simultaneous, independent testing of 16 devices.

## **THE INVESTIGATION ON BACK CONTACT INTERLAYER ZnTe, ZnTe/Cu, AND ZnTe/Cu<sub>2</sub>Te FOR CDTE SOLAR CELLS ON FLEXIBLE STAINLESS STEEL FOIL SUBSTRATES**

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Flexible stainless steel substrates have a promising future for thin film solar cells due to light weight, low cost, shape adaptability, and roll-to-roll manufacturing possibility. However, the poor conductivity of CdTe and poor contact between CdTe and Mo limited the efficiency because it is hard to generate an efficient ohmic back contact based on substrate configuration. The ZnTe band alignment with CdTe is favorable for hole transport and can be easily doped p+, and therefore easily contacted with a metal. In this poster, three ZnTe related interlayer materials, ZnTe, ZnTe/Cu, and ZnTe/Cu<sub>2</sub>Te were studied and compared. ZnTe was deposited on stainless steel substrates having a SiO<sub>2</sub> barrier layer by Closed Space Sublimation (CSS) and Mo bi-layer by RF sputtering. Cu and Cu<sub>2</sub>Te were both deposited by RF sputtering. Different thickness of Cu and Cu<sub>2</sub>Te were separately deposited on ZnTe. CdTe and CdS were also deposited by CSS. After CdCl<sub>2</sub> treatment, ITO was co-sputtered from SnO<sub>2</sub> and In<sub>2</sub>O<sub>3</sub> targets as the front contact. ZnTe did not show any improvement on the efficiency. Both thinner Cu and Cu<sub>2</sub>Te layer improved the “roll-over” of the I-V curve at the back contact. Accordingly, the fill factor and efficiency were also increased. Cu<sub>2</sub>Te doped ZnTe excelled Cu doped ZnTe because the controlling Cu diffusion.

## TRANSPARENT OXIDE/METAL/OXIDE TRILAYER ELECTRODE FOR USE IN TOP-EMITTING ORGANIC LIGHT EMITTING DIODES

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Organic light-emitting diodes (OLEDs) are emerging as the next generation, energy efficient display and lighting technology. Top-emitting OLEDs (TE-OLEDs) have the advantage of eliminating the substrate waveguiding modes existing in the more conventional bottom-emitting devices, and are compatible with active matrix display technology. The most commonly used transparent electrode, indium-tin oxide (ITO), is costly and requires methods of deposition that are highly destructive to the underlying organic layers. Here we have employed a trilayer electrode structure consisting of a thin layer of metal sandwiched between two MoO<sub>3</sub> layers, which can be deposited through vacuum thermal evaporation without much damage to the organic active layers. This MoO<sub>3</sub>/Au/ MoO<sub>3</sub> trilayer electrode was measured to have a maximum transmittance of nearly 90% at 600nm and a sheet resistance of 9 Ω/square with thicknesses of 5, 10, and 40 nm for the three layers. Using the trilayer as the top transparent electrode, we have fabricated green electrophosphorescent devices employing a p-i-n device structure with Ir(ppy)<sub>3</sub> doped in mCP as the emissive layer. Such a top-emitting device shows an external quantum efficiency of 11% and luminous power efficiency of 20 lm/W at 100 cd/m<sup>2</sup>, comparable with bottom-emitting devices using the same active layer structure and commercial ITO as the anode. The performance and emission characteristics of these devices indicate that this trilayer structure is a promising candidate as a transparent anode in top-emitting OLEDs.

## **EFFECT OF PROCESS PARAMETERS ON PROPERTIES OF MOLYBDENUM THIN FILMS FOR CIGS<sub>2</sub> THIN FILM SOLAR CELLS**

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Molybdenum back contact is deposited using DC magnetron sputtering. The properties of the thin film are dependant on the process parameters. Films deposited at high power and low pressure tend to be less resistive since the films are under compressive stress, however, such films exhibit poor adhesional strength. Films deposited at low power and high pressure tend to be under tensile stress and exhibit higher roughness and resistivity, while the film adhere very well to the sodalime glass substrate. Therefore, it has been a practice to deposit multi-layered Mo back contact to achieve the properties of good adhesion as well as low resistivity. As can be seen, the above mentioned process parameters and the corresponding film properties are at the two extreme end of the spectrum. Hence experiments are being carried out to optimize the sputtering power and pressure that will produce films that show acceptable properties of both the good adhesion and low resistivity. Efforts are being made to develop a single layered Mo film. Various combinations of sputtering power and pressure were experimented with. Tape test was done on each film to determine the adhesional strength of the films. The sheet resistance and the average roughness for each film were measured using a four probe measurement setup and the Dektak Profilometer, respectively. Moreover, atomic force microscopy (AFM) was carried out to determine the roughness of the film and X-ray diffraction (XRD) was carried out to determine the effect of process parameters on the crystallinity of the film. All the films considered in the figures have passed the tape test and, hence, can be concluded that the films exhibited good adhesion to the substrate.

## DEGRADATION OF OHMIC AND SCHOTTKY CONTACTS ON InGaAs HEMTs DURING STRESSING

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Numerous studies have shown that InGaAs based metamorphic high electron mobility transistors (MHEMTs) have similar mean time to failure (MTTF) as that of InP based HEMTs, about 10<sup>6</sup> hours. However, InGaAs MHEMTs require a substantial burn-in process in order to stabilize device performance and eliminate infant mortality. In order to study the device reliability and failure mechanisms, both high temperature storage tests and DC stress tests were performed on MHEMTs. MHEMTs were stressed for 36 hours at a drain voltage of 3V. Additional devices underwent a thermal storage test at 250°C for 36 hours. Transmission line method (TLM) structures were also stressed under similar conditions in order to isolate the effect of the gate on the device degradation. Under both stress conditions, the drain current decreased about 12.5%. The gate current, however, of MEHMT devices submitted to thermal storage increased much more than that of the devices subjected to DC stress. The main degradation mechanism observed for thermally stressed devices was reaction of the Ohmic contact with the underlying semiconductor. Devices stressed under DC suffered from substantial gate sinking, confirmed by transmission electron microscopy and energy dispersive spectroscopy.

## CUBIC $Zn_xMg_{1-x}O$ AND $Ni_xMg_{1-x}O$ THIN FILMS GROWN BY MOLECULAR BEAM EPITAXY FOR DEEP-UV OPTOELECTRONIC APPLICATIONS

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Oxide semiconductors have grown in interest in recent years for wide bandgap, deep ultraviolet optoelectronic applications.  $Zn_xMg_{1-x}O$  has seen extensive investigations, in part because of interest in wurtzite (B4) binary ZnO. Consequently, much of the investigation of  $Zn_xMg_{1-x}O$  has been focused upon the B4 crystal form, which realizes bandgaps in the range  $\sim 3.37$  to  $4.3$  eV and has greater Zn content ( $x$ ) than Mg. To realize deeper UV bandgaps ( $\sim 5 - 7.8$  eV), the ternary compound must be grown with higher Mg concentrations. In which it takes the rocksalt cubic (B1) crystal phase. While there exist some B1- $Zn_xMg_{1-x}O$  investigations, few have been upon lattice matched growth while still fewer have been carried out with plasma-assisted MBE on lattice matched substrates.

On the other hand,  $Ni_xMg_{1-x}O$  is a rocksalt ternary which has seen virtually no investigation in the single crystal, high-quality, thin film form. This material is also a direct wide bandgap ternary semiconductor that can realize bandgaps continuously from  $\sim 3.5$  eV to  $7.8$  eV, owing to the miscibility of NiO and MgO. Also of interest is the intrinsic p-type electrical character of  $Ni_xMg_{1-x}O$ , inherited from its binary parent NiO. NiO has recently been used as a p-type layer in conjunction with ZnO (which is intrinsically n-type) to realize p-n and p-i-n structures. However, the two materials have different equilibrium crystal structures, so these growths are not lattice matched and are therefore polycrystalline. A conjunction of the two compounds is logical due to the difficulty with p-type doping of ZnO (and similarly  $Zn_xMg_{1-x}O$ ).

We present the growth, characterization and application of  $Zn_xMg_{1-x}O$  and  $Ni_xMg_{1-x}O$  thin films grown by molecular beam epitaxy on approximately lattice matched MgO substrates. The points presented will include the lattice matching of the two ternaries and the aforementioned doping dichotomy. The successful application of both ternaries in metal-semiconductor-metal (MSM) implementations will be discussed and photoresponse measurements will also be shown. Significantly, we have successfully fabricated effective solar blind detectors from both material categories.

## EXTREME LUMINESCENT SIGNATURE OF COALESCED $\text{Cd}_x\text{Zn}_{1-x}\text{Se}$ QUANTUM-ROD ALLOYS

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Common ion semiconductor alloys in quantum structures such as dots and rods have the added benefit of control of the electron affinity of the material in addition to the fundamental spectral control provided by quantum confinement. Such alloys could be useful in mixed-material devices such as organic/inorganic photovoltaic cells, since inorganic valence and conduction energy levels can be appropriately matched to the HOMO/LUMO levels of the compatible organic phase. In this research we have synthesized common anion II-VI alloys consisting of a large band-gap core/small band-gap shell. We have been able to achieve a spectral signature ranging up to 200nm over the visible spectrum by a one-pot synthesis of  $\text{Cd}_x\text{Zn}_{1-x}\text{Se}$  alloys. The morphology of the alloy (supported by TEM, XRD and PL characterization) was a prolate rod-like quantum structure resulting from coalesced quantum dots consisting of three regions, each of which provides for a specific spectral signature. The 440nm PL peak was from ZnSe, while intermediate wavelengths were due to alloyed  $\text{Cd}_x\text{Zn}_{1-x}\text{Se}$ , and a peak at 640nm was due to a CdSe rich shell. With the judicious control of time and temperature of reaction, it was possible to create a multi-region quantum structure that mimicked the spectral characteristics of a selected alloy composition, i.e. achieve emission over a much larger range of the electromagnetic spectrum.

## EFFICIENT AND AIR-STABLE HYBRID ORGANIC-INORGANIC SOLAR CELLS BASED ON A LOW-GAP POLYMER AND CdSe NANOCRYSTALS

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Hybrid organic-inorganic solar cells based on conjugated polymers and colloidal inorganic nanocrystals have attracted significant attention as an alternative for all-organic solar cells. The incorporation of inorganic components in these solution-processed solar cells may possess additional advantages due to the high electron mobility and environmental stability of the inorganic materials. Here, we demonstrate efficient and air-stable hybrid solar cells using a low-gap polymer poly[2,6-(4,4-bis-(2-ethylhexyl)-4H-cyclopenta[2,1-b;3,4-b']-dithiophene)-alt-4,7-(2,1,3-benzothiadiazole)] (PCPDTBT) as the donor and spherical CdSe nanocrystals as the acceptor using the device structure of ITO/PEDOT:PSS/PCPDTBT:CdSe/ZnO/Al. PCPDTBT, with a bandgap of 1.55 eV, has strong absorption from ultraviolet to near infrared with an absorption edge of  $\sim 800$  nm. The hybrid active layer processed from chlorobenzene solution and annealed at  $150^{\circ}\text{C}$  shows somewhat percolated nanocrystals under transmission electron microscope, providing pathways for efficient electron transport. The devices using  $\sim 7$  nm CdSe nanospheres show a short-circuit current density of  $9.0\text{ mA/cm}^2$ , open-circuit voltage of  $0.76\text{ V}$ , fill factor of  $0.48$ , and power conversion efficiency of  $3.3\%$  under 1 sun AM1.5G illumination. The solution-processed ZnO nanoparticle layer between the hybrid active layer and the cathode acts as a hole-blocking layer and optical spacer, and leads to  $\sim 30\%$  increase in the power conversion efficiency of the devices. Furthermore, the devices with a ZnO layer maintained  $70\%$  of the original efficiency after stored in the air for over 60 days without any encapsulation, while the devices without a ZnO layer was completely degraded after several hours' exposure to the air.

## MANGANESE AND ANTIMONY TELLURIDE THIN FILMS FOR BACK CONTACT INTERFACES IN CdTe SOLAR CELLS

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Most metals, not having sufficiently high work functions necessary for being used as back contacts to Cadmium Telluride (CdTe) solar cells, form schottky barriers; and do not make good ohmic contacts [4].  $p^+$  metal tellurides as intermediate layers form a tunnel contact and are ideal for long-term cell performance [2].  $Sb_2Te_3$  is highly p-type and has a low resistivity of  $10^{-4} \Omega \text{ cm}$  [3] and its use as a good back contact interface have been proposed previously [1], [2], [3]. Manganese Telluride ( $MnTe_2$ ) and Antimony Telluride ( $Sb_2Te_3$ ) thin films are investigated for possible applications as good ohmic contacts to the CdTe foil based solar cells.  $MnTe_2$  thin films were formed using evaporation of  $MnTe_2$  at substrate temperatures ranging from RT to  $300^\circ\text{C}$ .  $MnTe_2$  based solar cells with  $V_{oc}$  of 530 mV and FF of 37% were achieved.  $Sb_2Te_3$  film formation was carried out in two ways: (1) Direct deposition of  $Sb_2Te_3$  by evaporation at substrate temperatures of 150 to  $350^\circ\text{C}$ . (2)  $Sb_2Te_3$  formation by deposition of Sb and Te and subsequent annealing.  $Sb_2Te_3$  based solar cells with  $V_{oc}$  of 580 mV and FF of 51% were achieved by direct deposition of  $Sb_2Te_3$ . Structural and electrical variations of  $MnTe_x$  and  $Sb_2Te_3$  films on cell performance are further being investigated.

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## NANOFORMULATION FOR THE TREATMENT OF MOLD

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Molds are microscopic fungi that grow in moist environment and use spores for reproduction. Molds can easily attack house/building materials such as dry walls, wood, grouts, carpet backing etc. Moreover, airborne mold spores can seriously compromise in-door air quality and can cause severe allergy, asthma and other immunological problems. Application of bleach has been very effective for the treatment of mold world-wide. However, action of bleach does not last long, requiring multiple applications. In our daily life we all experience how molds grow back in wet areas, specifically in the bathroom and kitchen, within a couple of weeks. In this poster, we examine the use of a silica based antibacterial/antifungal nanoformulation for preventing the spread of mold. The efficacy is tested using *Aspergillus niger*, a popular strain of mold used in industry testing.

## Polymer Translocation Induced by a Bad Solvent

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### Abstract

We implement Brownian Molecular Dynamics simulations on a homopolymer of lengths ranging from  $N = 16 - 256$  translocating through a nanopore, and study the effects of solvent quality (i.e. "good", "bad") asymmetries between the "cis" and "trans" compartments of the system on the translocation process. Specifically we study the "ratcheting" effect of a globule on the *trans*-side created on the translocated segment, and how this "ratchet" drives the system towards a quicker translocation. However, unlike the case of unbiased and forced translocation where the mean translocation time is characterized by single exponent  $\alpha$  ( $\langle\tau\rangle \sim N^\alpha$ ) and the histogram of the mean first passage time (MFPT) in reduced variable  $P(\tau/\langle\tau\rangle)$  exhibits scaling, we fail to notice such uniform scaling behavior for the entire translocation process. On the contrary, we notice a large  $N$  limit of  $\langle\tau\rangle \sim N^\alpha$  where  $\alpha \simeq 1$  for  $\epsilon/k_B T > 1$ . We also find that the translocation occurs with constant velocity attributed to the coiling of the globule. We argue that in absence of any external force, conservation principles dictate that the average translocation time should scale linearly with the chain length  $N$  in the large  $N$  limit.

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## LUBRICATION MECHANISM OF CARBON NANOONIONS DETERMINED FROM MOLECULAR DYNAMICS SIMULATIONS

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Nanostructured materials such as fullerenes and nanotubes have been of much interest to tribologists since the discovery of C<sub>60</sub>, buckminsterfullerene, in 1985. Within tribological systems, low friction coefficients are obtained for these nanostructured materials which are characterized by weak van der Waals (vdW) forces that govern the interactions. Understanding the lubrication mechanisms of nanostructured materials aids in determining their frictional properties as well as utilizing these materials in tribological applications. This presentation will report on the tribological behavior of carbon nanoonions (COs) both with and without a residual diamond core as a solid lubricant between two sliding, amorphous carbon surfaces. The molecular dynamics (MD) simulations presented here utilize the reactive empirical bond order (REBO) potential for short range interactions coupled with the Lennard-Jones (LJ) potential for long range vdW interactions. Through these MD simulations, the frictional behavior of the COs is found to be highly dependent on the interactions that occur between the fullerenes and the amorphous carbon surfaces. Without the presence of bond formations, the nanoonions are able to roll between the substrates provided extremely low frictional forces, but as bonds begin to form, the fullerenes are forced to slide which causes a significant increase in the observed friction. From these results, it has been shown that the lubrication mechanism of COs is a combination of rolling and sliding of the individual nanoonions at the sliding interface. The authors acknowledge the support of the National Science Foundation Grant No. CMMI-0742580.

## EVOLUTION AND STABILITY OF Pt-OXIDES ON SIZE-SELECTED Pt NANOPARTICLES

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The oxidation of Pt and the reactivity of Pt oxides are of fundamental importance in catalysis, and although much research has been conducted on the interaction of oxygen with Pt surfaces, most of the work is confined to UHV with bulk materials such as Pt(111). In this work we will explore the size-dependent oxidation and reduction properties of Pt nanoparticles (NPs) synthesized by reverse micelle encapsulation. We use in-situ O<sub>2</sub>-plasma treatments in conjunction with in-situ heating and X-ray photoelectron spectroscopy to monitor the temperature-dependent reduction of Pt<sup>δ+</sup> species in NPs with distinct size distributions. In addition, temperature programmed desorption was conducted to monitor the oxygen phases developed and the subsequent desorption profiles on these NP samples. These results are compared with the same experiments conducted on a Pt(111) single crystal.

## STRUCTURE AND PROPERTIES OF NICKEL/GRAPHENE INTERFACES

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Catalytic decomposition of hydrocarbons on transition metals is a common method to grow large areas of high quality of graphene. We study the atomic structure of graphene grown on Ni(111) by catalytic decomposition of ethylene at 600°C. Defects produced in graphene during epitaxial growth on Ni(111) substrate affects the electronic structure of graphene[1]. We have studied the atomic structures of defects produced in graphene using Scanning Tunneling Spectroscopy (STM). The point defects, which are in majority, can be due to Ni atoms embedded in graphene. We also have discovered for the first time extended line defects in graphene. These 1D structures are the consequence of domain boundaries between graphene-sheets occupying different registry relative to the nickel substrate. Atomic resolution STM showed that the line defect consists of fully  $sp^2$  hybridized carbon arranged in pentagons and octagons. Density functional theory showed that these defects have a high density of electronic states at the Fermi-level. The wavefunctions of these electronic states at the defect decay exponentially into the graphene lattice causing a local doping in the vicinity of the defect. This doping effect gives rise to the brighter contrast of the surrounding of the defect in STM images. Such atomic-scale wires have potential use for truly nanoelectronic devices build in graphene.

In another aspect of our work we investigate the interaction of Ni-supported graphene with Ni-adlayers. This study is motivated by the need of making metal contacts to graphene based electronic devices[2]. We deposited ~1ML of Ni on Graphene and studied the effect of annealing on the adsorbed Ni adatoms. Ni adatoms grow in 2D islands on a monolayer of graphene and forms 3D clusters on multiple layer graphene. During annealing 2D Ni islands intercalate beneath the Graphene. The intercalation process is not completely understood. It is a thermally activated surface diffusion process where the atoms penetrate under graphene through defects. During annealing Ni adatoms form a metastable  $Ni_3C$  which then decomposes at higher temperature and the Ni atoms intercalate.

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## ENHANCED PHOTOLUMINESCENCE OF $Gd_2O_3:Eu^{3+}$ NANOPARTICLES BY ENCAPSULATION WITH $Y_2O_3$

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$Gd_2O_3:Eu^{3+}$  nanoparticles were successfully synthesized and encapsulated by  $Y_2O_3$  with a facile polyol method. X-ray photoelectron spectroscopy (XPS) are consistent a mixture of  $Gd_2O_3:Eu^{3+}/Y_2O_3$  core/shell and  $Y_2O_3$  nanoparticles. The photoluminescence (PL) emission was from the  ${}^5D_0-{}^7F_2$  transitions of  $Eu^{3+}$  at 612 nm. Photoluminescent excitation (PLE) spectra showed that a small fraction of the emission from  $Eu^{3+}$  resulted from direct excitation, but the vast majority resulted from Oxygen to Europium charge-transfer excited between 225 and 275 nm for  $Eu^{3+}$  doped in  $Gd_2O_3$ . The encapsulated nanoparticles exhibited larger PL intensity than the  $Gd_2O_3:Eu^{3+}$  nanoparticles under the same conditions and the optimized nanoparticles with a  $Gd_2O_3:Eu^{3+}/Y_2O_3$  precursor ratio of 16:1 yielded PL intensity 20% higher than that of the  $Gd_2O_3:Eu^{3+}$  nanoparticles. All PL emission and excitation spectra were measured in drop-cast thin films which were a mixture of 20 mg of calcined nanoparticles in 500  $\mu$ L of PMMA.

**NOVEL SURFACE GRAFTING METHOD ON GLASS USING 3-(MERCAPTOPROPYL)TRIMETHOXY SILANE AS A COUPLING AND CHAIN TRANSFER AGENT**

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Silicate glass slides were surface-modified with homopolymers and copolymers using 3-(Mercaptopropyl)trimethoxysilane (MTS) as a combination silane coupling agent and chain transfer agent. The MTS was initially covalently bonded to an acid peroxide cleaned glass surface. The thiol end group of MTS functioned as the polymer chain transfer in aqueous solution. Polyacrylic acid (PAA), polyacrylamide (PAAm), polymethyl acrylate (PMA) and poly acrylamido-2-methyl-propanesulfonate (PAMPS) were grafted to the silylated surface. A poly(AA-co-AAm-co-MA-co-AMPS) was also prepared and characterized. Surface chemistry was characterized with attenuated total reflection fourier transform infrared spectroscopy (ATR-FTIR) and x-ray photoelectron spectroscopy (XPS). Surface texture was evaluated with atomic force microscopy (AFM). The wetting characteristics were measured with a sessile drop contact angle measurement. The results, to be presented, indicated successful grafting of each polymer and the copolymer onto the glass surface. The polymer-grafted surface, with a root mean square (RMS) roughness from 3.5 nm to 6 nm, was rougher than the acid peroxide cleaned surface, which had a RMS roughness of 0.7nm. This 3-step modification method is simple and cost-effective. A homopolymer or 4-component copolymer modified surface can be synthesized in a few hours.

**THEORETICAL AND EXPERIMENTAL STUDY OF THE HOMOGENEOUS  
THERMAL DECOMPOSITION OF THE TUNGSTEN DIMETHYLHYDRAZIDO  
COMPLEX  $\text{Cl}_4(\text{CH}_3\text{CN})\text{W}(\text{NNMe}_2)$**

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Continuing demands for the smaller integrated circuits, new diffusion barrier layers are needed to satisfy this trend. The use of copper instead of aluminum for the circuit interconnects makes circuit component size smaller. Although replacing aluminum with copper as interconnect material increases current speed, a diffusion barrier material is needed to protect the interaction between copper and Si because copper has high diffusivity into Si. For this purposes, various candidates such like Ta, Ti or W-based materials have been studied. Among these, W-based material shows good performance based on the efficacy advantage of  $\text{WN}_x\text{C}_y$  as a diffusion barrier. To achieve better film properties, various W-based precursors have been designed, explored and tested, and tungsten dimethylhydrazido complex has been chosen for this research. The decomposition kinetics of dimethylhydrazido tungsten complex  $\text{Cl}_4(\text{RCN})\text{W}(\text{NNMe}_2)$  (**1a**,  $\text{R}=\text{CH}_3$  and **1b**,  $\text{R}=\text{Ph}$ ), a novel precursor for single source deposition of Cu diffusion barrier, was designed and synthesized and then has been examined in a vertical upflow, cold-wall CVD reactor by in situ Raman spectroscopy.

In situ Raman experiments were performed using a susceptor set point temperature 850°C and liquid benzonitrile measurement was also performed for excluding solution effect. Due to the low concentration of title compound, signals were relatively weak, however, reasonable signal to noise ratio was obtained with repeated scan and longer detection time.

From main experiments, features at 1177.5, 1189, 1193, 1247, 1638, 2242, 3377, 3426 $\text{cm}^{-1}$  were measured and assigned. The results of Density Functional Theory (DFT) calculations were used to describe the decomposition behavior and assign the observed Raman bands (1177.5  $\text{cm}^{-1}$ , 1189  $\text{cm}^{-1}$ , 1193  $\text{cm}^{-1}$ , 1247  $\text{cm}^{-1}$ , 1638  $\text{cm}^{-1}$ , 2242  $\text{cm}^{-1}$ , 3377  $\text{cm}^{-1}$ , 3426 $\text{cm}^{-1}$ ) of reaction intermediates to the decomposition products such as dimethylamine (DMA), monomethylamine (MMI),  $\text{H}_2\text{NWCl}_4$ , etc. Except those peaks, although five other peaks were detected, it could not be assigned properly. From in situ Raman spectroscopy experiment and DFT calculations, both W-N1 and N1-N2 cleavages are possible although N1-N2 cleavage is favorable energetically and both cleavages would produce dimethylaminyl radical.

DFT calculations using B3LYP/LanL2DZ model chemistry were performed to build full reaction mechanism and screen possible decomposition routes and estimate their reaction rate parameters. We confirmed decomposition process follows energy favorable path from detected materials and constructed reaction schemes by DFT calculations.

## EFFECT OF DOPANTS ON THE STABILITY OF TRANSIENT PHASES FORMED DURING CRYSTALLIZATION OF SOLUTION DEPOSITED PZT THIN FILMS

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Lead zirconate titanate thin films have potential application in pulsed discharge capacitors due to their high dielectric constant. Solution deposition is a standard route for fabricating these thin films. In solution deposition, the precursor solution is first deposited on the substrate to form an amorphous film. The amorphous film is crystallized by heating it at a high temperature (~600-650°C). During crystallization various transient phases, such as  $Pt_xPb$  and Fluorite type phase, are formed. These transient phases influence the final properties obtained in these thin films. Although aliovalent doping of PZT is routinely undertaken to enhance the properties of PZT, the effect of these dopants on the stability of the transient phases has not been systematically studied. To study the effect of dopants on the stability of transient phases, we chose an A-site dopant (La) and a B-site dopant (Nb). To observe the effect of the dopants on the transient phases, thin films of doped PZT composition were crystallized by heating to 600°C at 5°C/min. Diffraction patterns of the thin film samples were simultaneously collected during crystallization to characterize the different phases formed at different temperatures and times. Diffraction peaks of the different phases observed during crystallization were peak fit using MATLAB with a Pearson-VII type function in which the contribution of  $K\alpha_1$  and  $K\alpha_2$  were included. The integrated intensities of different phases were plotted against time, providing the time and temperature dependence of the evolution of different phases. In comparison to un-doped PZT, Nb-doping was found to decrease the temperature range over which the  $Pt_xPb$  is observed by ~10°C. The temperature range over which the fluorite phase was observed was shifted by ~10°C in Nb-doped thin films. Nb-doping also effected the formation of the final perovskite phase. Although the temperature/time at which the perovskite phase is formed observed was lower for Nb-doped PZT, the time/temperature at which the film completely crystallized into a perovskite phase was higher by ~34°C. The results presented in the poster will include the studies on La-doped PZT thin films, which are currently underway. The obtained results will be discussed with respect to the current understanding of phase evolution.

## MODELING CdTe/CdS THIN FILM CELLS USING SCAPS-1D

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A large bandgap of 1.45eV and a high absorption coefficient make CdTe a prime candidate for solar cells. Producing these cells on flexible foil increases their advantages even more by making them lightweight and also enables them for roll-to-roll manufacturing.

In order to understand various effects in these cells, a device simulation software - SCAPS-1D - developed by the University of Gent, is being used. This tool enables one to vary different parameters, like doping levels, defect densities, series and shunt resistance, etc. It also enables one to study different structure combinations. Our focus is to model the CdTe/CdS solar cell in the substrate configuration, as we consider building these cells on flexible foil, under ideal conditions. Subsequently, parameters will be varied to study their impact, including interface defects and traps, to match their performance to the characteristics of cells fabricated in our lab. Some of the effects are the back contact diode causing a roll over in the IV curve, and current loss due to recombination sites at the interfaces and within the layers. This paper will review our findings on the impact of various material and device characteristics on solar cell performance.

## HYDROCARBON DEPOSITION ON POLYMER SURFACES

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Ion beam deposition is a common method used in modification of polymer surfaces. However, the chemical mechanisms inherent in this process are not well understood, due to the difficulty of experimental characterization. Therefore, molecular dynamics simulations were carried out using the second-generation reactive empirical bond-order (REBO) potential developed by Brenner and co-workers. Hydrocarbon ions C, CH<sub>2</sub> and C<sub>2</sub>H were deposited on poly(methyl methacrylate) and polystyrene. Thermal deposition energies ranging from 4eV to 50eV were used. Products were categorized as a function of energy and ionic species in order to determine the optimum deposition conditions to induce a desired chemical reaction.

## IMPACT OF GAUSSIAN SCATTERERS ON TRANSPORT PROPERTIES OF GRAPHENE

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We have measured the impact of atomic hydrogen adsorbates on transport properties of graphene sheets as a function of adsorbate density at 15 K in ultra high vacuum environment. Only charge neutral atomic hydrogen was introduced in our experiments by using custom ion deflector. Atomic hydrogen on graphene behaves as weak Gaussian scatterers with their impact radically different from those of coulomb scatterers. Importantly, atomic hydrogen impurities do not drive graphene into the insulating state even at saturation. This result is surprising as atomic hydrogen has been expected to introduce highly disruptive short-range scattering. We will discuss our results in context of recent calculations, which consider more realistic scattering potential exerted by atomic hydrogen, the effect of dipole at the hydrogen carbon bond and the impact of other extrinsic factors not varied in our experiments.

**INFRARED ABSORBANCE OF MINERAL POWDERS:  
CORRECTIONS BASED ON PARTICLE SIZE DISTRIBUTION**

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Far-infrared absorption spectra of mineral powders bear characteristic features that can be used to interpret emission spectra of astrophysical dust populations. We are collecting such mineral spectra in support of the Herschel Space Observatory data return. To avoid saturation of the absorbance, the effective thickness of the mineral samples must be less than a few microns, and this is best achieved by dispersing micron-size mineral particles in a polyethylene host. If particle sizes exceed the effective thickness, then the absorption coefficients derived from the data will be quantitatively inaccurate. This paper presents a method of correcting the absorption spectra for actual particle size distributions determined from scanning electron microscopy.

## **IN-SITU STRAIN MEASUREMENTS OF EB-PVD THERMAL BARRIER COATINGS USING SYNCHROTRON X-RAY DIFFRACTION UNDER THERMO-MECHANICAL LOADING**

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Demands for designing prime reliant, energy-efficient, and high-performance thermal barrier coatings (TBCs) in gas turbines have led to a growing interest toward comprehensive microstructural characterization. Over the last decade, Synchrotron X-ray Diffraction (XRD) has established itself as a high-resolution strain measurement method for the thermally grown oxide (TGO) layer of thermal barrier coatings (TBCs). With recent advances in the development of in-situ load and thermal instrumentation at the synchrotron beamline, operational environments of jet engine turbine blades can be more accurately replicated. In this work, we present in-situ x-ray strain measurements of the TGO layer on cycled TBC specimens under thermo-mechanical loading using powerful high energy x-rays (~80.7-86 keV) at Sector 1-ID of the Advanced Photon Source at the Argonne National Laboratory. The evolution of TGO stresses was examined over one complete thermal cycle on TBC samples at various stages of the life fraction.

## EFFECTS OF ALLOYING AND DOPING IN SEMICONDUCTOR NANOWIRES: $\text{Cd}_x\text{Zn}_{1-x}\text{S}:\text{Mn}$ , A CASE STUDY

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Synthesis of semiconductor nanowires requires special synthesis condition to guide growth in one-dimension. Making alloy semiconductor introduces additional constraints in the growth environment. The success of the experiments depends on several parameters such as suitable choices of the elementary components, response of these elements to the growth environment, lattice strain etc. Most of the semiconductor materials tend to oppose to the impurity doping during their crystal growth due to self-purification phenomena. Thus in order to achieve desired doping, the growth condition needs to be tuned to enhance impurity doping. In the present work we have successfully fabricated ternary alloy semiconductor  $\text{Cd}_x\text{Zn}_{1-x}\text{S}$  nanowires by a simple synthesis routes. Moreover we have successfully tailored the growth environment to incorporate the transition metal ion  $\text{Mn}^{2+}$  into these alloy nanowires. We have observed development of various new morphological and optical phenomena related to alloying and doping. Alloying leads to the formation of self-assembled three dimensional urchins which consisted of nanowires. Detail investigation shows that strain induced in the crystal due to ionic radii mismatch of the two cations produced structural defects in the nanowires. These defect sites served as the secondary nucleation sites for the formation of three dimensional assemblies of nanowires. It was observed that Mn doped samples could exhibit yellow emission at room temperature for  $x \leq 0.65$ .

## ATOMIC FORCE MICROSCOPY STUDY OF COLOSSAL MAGNETORESISTIVE OXIDE THIN-FILM SURFACE ROUGHNESS

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Complex oxides are the subject of intense research due to the wide variety of behaviors they display, including drastic changes in its metallic properties when exposed to weak magnetic fields, known as colossal magnetoresistance (CMR). The physics behind this phenomenon is still under debate, but the roughness of the material is known to affect it. In this project, the morphology of the CMR oxide lanthanum strontium manganite (LSMO,  $\text{La}_{0.65}\text{Sr}_{0.35}\text{MnO}_3$ ) has been studied using atomic force microscopy (AFM). The principles of the AFM itself have been learned and applied. A basic understanding of thin film growth was required in order to correlate surface morphology to epitaxial growth modes. The basics of the synthesis equipment, off-axis radio frequency (RF) magnetron sputtering, were learned. Thin film growth was optimized by observing the quality of the films obtained under different growth conditions. 27 samples were analyzed and over 250 images taken, which provided interesting results. Two samples showed a difference in roughness at different locations. Substrate-induced strain was studied by growing the LSMO on different substrates; namely, strontium titanate (STO,  $\text{SrTiO}_3$ ) and lanthanum aluminate (LAO,  $\text{LaAlO}_3$ ). Scanning at different degrees did not demonstrate significant differences in measurements. A graph of roughness vs. film thickness shows a similar trend with both substrates, with LAO having a larger average roughness. These results provide a starting platform for future research on LSMO, which may include growing at different thicknesses on STO and LAO or growing on different substrates with different lattice constants.

## **DIFFUSION BARRIER STUDY FOR CDTE SOLAR CELLS ON FLEXIBLE STAINLESS STEEL FOIL SUBSTRATES**

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It was found that the out diffusion of impurities, such as Fe and Cr from stainless steel substrate into CdTe cell is detrimental. Especially after the CdCl<sub>2</sub> treatment, the chemical reaction between Cl and Cr or Fe drives them out of the surface. Two diffusion barrier materials, Si<sub>3</sub>N<sub>4</sub> and SiO<sub>2</sub> were investigated. Both Si<sub>3</sub>N<sub>4</sub> and SiO<sub>2</sub> barriers were deposited on oxidized stainless steel (SS430) foil substrates at room temperature by RF sputtering. However, Si<sub>3</sub>N<sub>4</sub> deposition was done in Ar ambient from a Si<sub>3</sub>N<sub>4</sub> target and SiO<sub>2</sub> barrier was deposited by reactive sputtering from a Si wafer in Ar (50% in volume) and O<sub>2</sub> ambient. Different thickness of barrier was investigated and compared. Standard CdTe/CdS cells were fabricated on stainless steel, Si<sub>3</sub>N<sub>4</sub> or SiO<sub>2</sub> coated stainless steel foil substrates. It's concluded that 1 μm SiO<sub>2</sub> is thickness enough to block most of the impurity. The efficiency of cells with barrier was highly improved. The highest efficiency obtained from a standard cell with a SiO<sub>2</sub> barrier was 6%. Industry standard ASTM D3359-08 tape test was used to characterize the adhesion of different cells and found out that barriers did not degrade the adhesion. On the contrary, the adhesion of cells without barriers was worse due to impurity diffusion. And, both diffusion and blocking of impurities in the cell was demonstrated by EDS map of line at the cross section of every cell.

## SURFACE STRUCTURE DEPENDENT NUCLEATION AND DESORPTION OF ACETIC ACID ON RUTILE TiO<sub>2</sub>(110) AND (011)-(2×1) SURFACES

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We present a combined experimental and theoretical study of the adsorption and desorption of acetic acid on the rutile TiO<sub>2</sub>(110) and (011)-2×1 surfaces. The different atomic structure of these two surfaces gives rise to strong face dependent adsorption behavior. Using scanning tunneling microscopy (STM) the adsorption structure of acetate is studied on the two surfaces. Only monodentate adsorption of acetic acid on TiO<sub>2</sub>(011)-2×1 surface is predicted. Density functional theory (DFT) calculations indicate that acetic acid adsorbs only weakly on the TiO<sub>2</sub>(011)-2×1 surface, while hydroxyl (-OH) groups at surface stabilize the adsorption through H-bonding. The H-bonding with a surface -OH group increases the adsorption energy to 0.84 eV/molecule. With the assistance of the H-bonding with surface -OH group and inter-molecular H-bonding, acetic acid clusters are formed on TiO<sub>2</sub>(011)-2×1 surface at higher coverage that are confined along [0-11] direction. On rutile TiO<sub>2</sub>(110) surface, acetate adsorb strongly in a bidentate adsorption configuration and STM shows the formation of a single well-ordered superstructure with a (2×1) periodicity at saturation coverage. The different adsorption behaviors are strongly related to their distinct chemical environment of the surface fivefold Ti (Ti<sub>5c</sub>) atoms. However, the temperature programmed desorption (TPD) measurements suggest that the different bonding geometries play only a minor role for the thermal reaction mechanism. Adsorbed acetate reacts to form ketone as the major desorption product at about 600 K, independent of the surface orientation.

## SIMULATIONS OF THE AGING MECHANISMS FOR AMORPHOUS CERIUM DIOXIDE USING DENSITY FUNCTIONAL THEORY

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Amorphous Cerium dioxide prepared from  $\text{CeCl}_3$  and NaOH in the presence of  $\text{H}_2\text{O}_2$  undergoes aging process as evidenced by discoloration. We propose that the aging mechanism involves several intermediates formed through the oxidation of  $\text{Ce}^{3+}$  to  $\text{Ce}^{4+}$ . Here we investigate the structures and thermodynamics of the complexes formed by Cerium with water and hydrogen peroxide using Density Functional Theory. Different variations of the Cerium complex were used to study the oxidation patterns of the two Cerium atoms as well as electron transfer from antibonding orbitals to Ce f-orbitals. We look at the energies as an indicator of the electronic configurations of the intermediate structures. We found the complex with two  $\text{Ce}^{4+}$  atoms surrounded by water ligands and hydroxyl groups and bridged by peroxide and hydroxyl groups to be the most stable (Figure 1). Predictions on kinetics of the aging process are also made.

Undergraduate: Computational and Experimental Materials Science

## USE OF COLD PLASMA FOR THE SURFACE MODIFICATION OF THE NATURAL POLYMER XANTHAN

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A hybrid reaction system consisting of an atmospheric-pressure plasma chamber coupled with a fluidized-bed reactor was used to modify the surface of the biopolymer xanthan. For this purpose a powder of xanthan was fed to the reaction chamber and was fluidized before being exposed to a helium atmospheric-pressure plasma in order to induce the generation of free radicals in the surface of the particles. Afterwards, the biopolymer received an in-situ treatment consisting on the exposure to epichlorohydrin vapors in order to generate oxirane groups on the surface. The presence of these groups facilitated the formation of covalent bonds when the xanthan was used to make biohydrogels chitosan/xanthan. When using untreated xanthan, the biohydrogel it is not mechanically stable due to the ionic characteristics of the bonding between the two biopolymers. Different treatment conditions were used in order to control the amount of oxirane groups, which in turn control the density of covalent bonds, and therefore it is possible to tailor the swelling capabilities of the hydrogel depending on the application.

**MULTI-TECHNIQUE SURFACE ANALYSIS OF ORGANIC LED PRECURSOR FILM**

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Liquid crystal displays have been with us for many years now and many people have replaced their CRT-based TVs with larger, high definition compatible LCD screens. In the future, it is expected that screens based on organic LEDs will replace these units. OLED displays typically draw less power than LCDs, since the backlights required for LCD screens are not needed. As a result, portable screens can run for longer from a single battery charge.

A possible OLED material is poly (9, 9-dioctylfluorene), which is more simply known as PFO. PFO is a high brightness blue-light emitting material with a low turn-on voltage and great potential for the future. It has a large optical gap, however, and that means that in order to make the most of its potential for OLED displays, the overall design of the OLED device has to be carefully developed and controlled to prevent any adverse interaction with charge carriers in PFO films.

To understand the interaction of PFO with charge carriers, it is necessary to understand the electronic structure of PFO itself. This requires a multi-technique analytical approach. Thermo Scientific offers XPS tools which can be configured with multi-technique options, allowing much of the electronic structure of PFO to be investigated with a single instrument.

## CELL ADHESION BEHAVIORS ON MICROPATTERNED SUPER-HYDROPHOBIC/SUPER-HYDROPHILIC SURFACE

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In this presentation, we report the adhesive properties of NIH 3T3 fibroblast cells on micropatterned super-hydrophobic/super-hydrophilic surface. The super-hydrophilic surface used in this study has roughness structures that can strongly affect the cell adhesion properties as well as the super-hydrophobic surface. The effects of the distances between patterned regions and physicochemical properties of the surfaces such as roughness and wettability on cell adhesion are also presented. The physicochemical properties of the super-hydrophobic and super-hydrophilic surfaces are reviewed by water contact angle measurements, atomic force microscopy (AFM), Kelvin force microscopy (KFM), field emission scanning electron microscopy (FESEM), environmental scanning electron microscopy (E-SEM), and X-ray photoelectron spectroscopy (XPS).

Super-hydrophobic films were deposited on Glass plates or Si wafer substrates using microwave plasma enhanced chemical vapor deposition. The raw materials were a gas mixture of trimethylmethoxysilane (TMMOS) and Ar. The partial pressures of TMMOS and Ar were kept constant at 27 and 40 Pa, respectively. After film deposition, vacuum ultraviolet (VUV) light at a wavelength of 172 nm irradiated the substrate for 30 min at a pressure of 10 Pa through a photomask to fabricate a super-hydrophilic region. Mouse 3T3 fibroblast cells were cultured using Dulbecco's modified Eagle's medium (DMEM) supplemented with 10% Fetal Bovin Serum (FBS), 0.2 mg/ml streptomycin sulfate, and 100 U/ml potassium penicillin G. These cells were cultured at 37 °C in a humidified atmosphere of CO<sub>2</sub> and 95 % air.

When the cells were seeded on the micropatterned super-hydrophobic/super-hydrophilic substrate, the cells attached to the super-hydrophilic regions in a highly selective manner, forming circular arrays corresponding to the pattern.

## LASER TREATMENT EFFECTS ON FIELD EMISSION PROPERTIES OF SINGLE-WALLED CARBON NANOTUBE BUCKYPAPERS

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Many researchers regard carbon nanotube backlight units (CNT-BLUs) as a potential candidate for the liquid crystal display (LCD) industry. CNT buckypapers were tested as surface luminary sources for CNT-BLU applications. The field emission properties, durability and repeatability of a single-walled Carbon nanotube (SWCNT) buckypaper was studied for developing CNT-BLU. This study reports a laser irradiation process to modify the surface of buckypaper and enhance the field emission properties. A scanning laser treated selected regions of the buckypaper to activate CNT emitters. This post-process causes a decrease in turn-on field and increases in the field enhancement factor ( $\beta$ ), luminance intensity and uniformity of buckypaper emitters. The phosphorescence luminance intensity and uniformity of buckypaper emitters were measured and characterized. These excellent properties and performance were achieved by adjusting machining parameters of laser power, laser lens motion speed, laser resolution. Design of Experiment (DOE) methodology provided a method to rapidly search the feasible laser parameter setting for processing buckypaper and improving field emission properties within fewer experimental runs. DOE results indicated the proper laser treatment power density was  $0.9 \text{ W/cm}^2$ . Furthermore, the effects of the laser treated emitter density was investigated under the same laser power density as the DOE results. The CNT emitter's altitude, diameter and spacing were characterized through an optics analysis after laser treatment. The emitter spacing directly impacted emission results when the laser power and treatment time were fixed. The increasing emitter density gave rise to an enhanced field emission current and luminance. However, a continuous and excessive increase of emitter density with spacing reduction generated a screening effect. As a result, the extended screening effect from the smaller spacing eventually crippled the field emission effectiveness. From luminance intensity and uniformity of field emission, the optimal ratio of average emitter altitude to emitter spacing was 3.4. The high effective buckypaper is suggested to have a density of  $50 \times 50$  emitters/ $\text{cm}^2$ , which presents an effective field enhancement factor of 3721 and a moderated screening effect of 0.005. Proper laser treatment appears to be an effective post-treatment process for optimizing field emission and luminance performance for a buckypaper cold cathode.

## OPTIMAL DEPOSITION CONDITIONS AND CHARACTERIZATION OF ALUMINUM OXYNITRIDE FILMS DEPOSITED BY ION BEAM SPUTTERING AT ROOM TEMPERATURE

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Aluminum oxynitride films were deposited by ion beam sputtering deposition (IBSD) at room temperature. Three different gases, nitrogen, oxygen, and argon, were used during different deposition processes in order to find the optimal deposition conditions such as ion beam voltage and oxygen partial pressure ( $P_{O_2}$ ) to fabricate aluminum oxynitride films. The optical properties (transmittance, refractive index, and extinction coefficient), film morphology (surface roughness) and structural properties (crystallinity, relative concentration and chemical bonding environment) of the aluminum oxynitride films were investigated by UV/visible/near IR spectrometer, atomic force microscopy, x-ray diffractometer, and x-ray photoelectron spectroscopy (XPS). Even though many studies were reported previously this is the first time a sequential film deposition with different gases was used to determine the optimal deposition parameters for aluminum oxynitride films. The properties of the films as functions of oxygen partial pressures demonstrate that the optical properties and surface roughness can be tailored by adjusting the ratio of oxygen to nitrogen partial pressure during the deposition. Aluminum oxynitride films were amorphous with three aluminum oxynitride networks,  $AlO_2N$ ,  $AlO_{2.5}N$  and  $AlO_3N$ , as the oxygen partial pressure increasing.