Energy

X Functional materials for environmental sensors and energy systems

About three quarters of the European population lives in urban areas. The urban environment has a profound effect on people's health and well-being. Environmental sustainability and energy efficiency of the urban society is a key issue in the era of smart cities and information services for the quality of life. Solid state sensors and energy systems based on advanced functional materials have been developed for several decades and recent improvements in nanotechnology and multifunctional materials have open up the possibility to develop a new generation of sensitive, selective and stable sensors integrated in autonomous systems, with largely improved capacity and enhanced performance to give relevant information both on a personal level and systems level.

Scope:

Air quality takes a prominent position in discussions on urban environment and health, and it is a concern for many inhabitants of urban areas. Nanotechnologies, including nanostructured materials for sensing, chemical sensors, portable systems and commercial devices, give a challenging opportunity to create a new generation of sensor-systems for air quality control and efficient energy systems. Functional nanomaterials (i.e., nanowires, nanotubes, graphene, nanoparticles of metal-oxides, carbon-nanostructures, large band-gap semiconductors, and metals) with new sensing properties (detection at ppb-level, high sensitivity and selectivity), self-heating and durable operations for low-powered (tens of □Watt to tens of mWatt) devices are key elements in air quality measurements at indoor and outdoor level.

Piezoelectric and/or thermoelectric materials are crucial for developing autonomous devices to be integrated in efficient stand-alone systems for energy harvesting. Advanced materials for energy applications are key enabling technologies in the field of energy efficiency and energy saving.

Modeling provides a tool for nanomaterials tailor-made for specific purposes and applications. In order to realize functional improvements in packaging, both testing and aging investigations are also very important and a focus area of this symposium as current research hot-issues.

Nanotechnologies offer a big challenge to create innovative low-cost sensors for air quality monitoring and energy systems applications. Functional nanomaterials (one- and two-dimensional nanostructures of carbon, graphene, metal-oxides, metals, polymers, supramolecular materials, self-organized materials, organic/inorganic materials, hybrid composites) with new tailored properties are key-issues for the development of low-powered devices for indoor and outdoor air quality monitoring, including practical applications such as geo-tagged database collected by networked stationary or mobile smart devices to address new sensing concepts for air quality monitoring and mapping techniques of gas molecules and particulate matter. These solid-state chemical sensors based on smart materials with autonomous operation and low-power consumption are useful for a real deployment and complementary to the existing official high-cost accurate air-quality monitoring stations used by public authorities. These new cost-effective sensor-systems will be beneficial for science community, policy makers and social networks.

Many worldwide investigators are involved in research in materials physics/chemistry and engineering, including nanosciences and nanotechnologies for chemical sensing and energy applications. Current international research includes the design and synthesis of organic, inorganic, polymers, and hybrid materials, the development of biomimetic materials and biomaterials, the discovery of new organometallic catalysts, the synthesis of nano- and mesoscopic materials including raw materials, the preparation of multilayers and multifunctional coatings, the study of chemistry of surfaces and interfaces, the exploration of the sensing properties of reactive materials, the characterization of the matter at nanoscale level for deep insights, the photo-physical study of supramolecular materials, the investigations of the new piezoelectric and thermoelectric materials for energy harvesting, and the demonstration of functional nano/micro systems.

Basic research on sensing mechanisms and gas/surface interaction, including new effects and concepts, is critical for advancements in materials science and sensors in order to address practical applications in the field of the environmental monitoring, energy efficiency, safety, security, healthcare, automation, green buildings, transportations, food quality, industrial process control.

Hot topics to be covered by the symposium:

The specific scientific and technological areas are:

- Advanced gas sensing semiconducting materials
- Hybrid materials and nanocomposites for chemical sensing
- Catalytic sensing materials
- Metal oxides for chemical sensing and/or energy applications
- Carbon-based materials for chemical sensing and/or energy applications
- Piezoelectric and/or thermoelectric materials for energy harvesting applications
- New nanotech sensors for monitoring gaseous and liquid pollutants

- Surface-sensitive spectroscopies for studying sensor/gas interaction
- Modeling of materials, devices, sensor systems and energy systems
- Functional applications of environmental sensors and/or energy systems

START AT	SUBJECT	View All	NUM.	ADD

Welcome address : Michele Penza

13:45 Welcome address **X.0.1**

Authors : Michele Penza1, Anita Lloyd Spetz2, Meyya Meyyappan3, Albert Romano-Rodriguez4
Affiliations : 1 ENEA, Italy 2 Linköping University, Sweden 3 NASA, USA 4 Universitat de Barcelona, Spain

Resume : Welcome address

Metal Oxide Nanostructures for Gas Sensing I : Albert Romano-Rodriguez

14:00 Uniform Metal-Oxide Semiconductor Multilayer Porous Thin Film for Enhanced Gas Sensing Performance **X.I.1**

Authors : Pingping Zhang, Shumin Zhang, Hui Zhang, Xuhui Sun*
Affiliations : Institute of Functional Nano & Soft Materials, Soochow University

Resume : Highly-uniform bilayer and multilayer porous thin films were successfully fabricated using self-assembled soft template and simple sputtering deposition technique. The sensor based on the In2O3/CuO bilayer porous thin film shows obviously improved sensing performance to ethanol at the lower working temperature, compared to single layer counterpart sensors. The response of In2O3/CuO bilayer sensors exhibit nearly 3 and 5 times higher than those of the single layer In2O3 and CuO porous film sensors over the same ethanol concentration, respectively. The sensing mechanism based on p-n hetero-junction, which contributed to the enhanced sensing performance was also experimentally confirmed by a control experiment which the SiO2 insulation layer was inserted between the In2O3 and CuO layers to break the p-n junction. In addition, the sensing performance can be further enhanced by increasing the number of In2O3/CuO junction layers. The facile process can be easily extended to the fabrication of other semiconductor oxide gas sensors for practical sensing applications.

14:30 Semiconductor oxide surfaces modified by laser interference lithography (LIL) for pollutant detection **X.I.2**

Authors : L. Parellada, I. Castro-Hurtado, E. Castaño, G.G. Mandayo
Affiliations : Ceit and Tecnun (University of Navarra)

Resume : Metal oxide semiconductors and their different nanostructured forms have been widely researched in the last years. They show high interest to fabricate cheap chemoresistive gas sensing devices. Materials like ZnO, SnO2, In2O3 or TiO2 are well known for their cost-effectiveness, fast response and high sensitivity when exposed to target gases. As it is well known, chemoresistive gas sensors rely on the electric response caused by the gas on the material surface. The grain size and morphology of the

material are also of great relevance in the gas sensing mechanism. Therefore, research efforts are focused on finding easy-to-implement and efficient fabrication routes, which at the same time give rise to an optimum morphology. In particular, several routes have been researched to obtain nanostructures. Some of them are bottom-up methods, such as the chemical vapor based routes such as the VL (vapor-liquid) or the VLS (vapor-liquid-solid) methods, widely reported to obtain nanowires, nanoneedles, nanobelts and other similar one dimensional nanostructures. But there are also some interesting top-down routes such as e-bean lithography or nano-imprint lithography. Among those, laser interference lithography is a technique that uses interference patterns generated from two or more coherent laser beams to structure materials. One of its advantages is that the material processing is fast, repeatable and can be applied at wafer level during the fabrication process of the sensing devices. In this work, zinc oxide sputtered thin films have been processed on alumina substrates using the laser interference lithography tripled Q-switched Nd:YAG laser source with an output wavelength of 355 nm. The aim is to obtain periodic structures on the surface, varying the process conditions in order to increase the surface area of the devices but also to modify the morphological properties of the devices and study their influence on the gas sensing properties of ZnO. The structural characterization has shown that the material changes its morphological properties and two-dimensional patterns have been obtained and implemented in gas sensing devices (including interdigitated electrodes and a back-side heater). Their gas sensing behavior is being researched and compared to the thin film ZnO oxide. Preliminary results show response enhancement in some of the obtained structures.

14:45 Site-specific growth of nanostructured oxides for sensing applications **X.I.3**

Authors : S. Barth1, L. Hrachowina1, J. Sama2, G. Domenech-Gil2, I. Gracia3, C. Cane3, A. Romano-Rodriguez2
Affiliations : (1) Vienna University of Technology, Institute of Materials Chemistry, Getreidemarkt 9, A-1060 Vienna, Austria; (2) Universitat de Barcelona (UB), MIND-Departament of Electronics and Institute of Nanoscience and Nanotechnology (IN2UB), c/Martí i Franquès 1, E-08028 Barcelona, Spain; (3) Consejo Superior de Investigaciones Científicas (CSIC), Institut de Microelectrònica de Barcelona (IMB-CNM), Campus UAB, E-08193 Bellaterra, Spain

Resume : Nanostructured, porous oxides are prominent sensing materials due to the reversible change in resistivity upon changes in the surrounding atmosphere. Nanowires have gained considerable attention in gas sensing devices due to their high surface to volume ratio and high crystallinity. However, the cost effective integration of nanowires in functional devices is usually challenging and costly. We present a cost effective and simple growth strategy using CMOS-compatible micromembranes containing a buried heating element, which is used for thermally induced chemical vapour growth of tin and tungsten oxides as well as the heating source for the effective operation as sensor. The small membrane volume and area requires low power (few mW) for both the growth and the operation of the resulting devices. The actual device contains a porous network of nanowires bridging interdigitated electrodes on top of the membrane for the electrical readout. Secondary deposition products should be negligible, which can be demonstrated by cross-sectioning of the active part of the device. The devices have been successfully used in monitoring changes in CO and ammonia concentrations and show long-term stability.
References: [1] S. Barth, R. Jimenez-Diaz, J. Sama, J. D. Prades, I. Gracia, J. Santander, C. Cane, A. Romano-

Rodriguez. Chem. Commun. 2012, 48, 4734. [2] J. Sama, S. Barth, G. Domenech-Gil, J. D. Prades, N. Lopez, O. Casals, I. Gracia, C. Cane, A. Romano-Rodriguez, submitted.

15:00 ZnO nanorod p-n junction piezoelectric energy harvesters for self-powered wireless sensor nodes **X.I.4**

Authors : Joe Briscoe
Affiliations : Materials Research Institute, Queen Mary University of London, UK

Resume : Oriented films of ZnO nanorods can be coated easily using low temperature solution methods onto a wide range of substrates, including flexible plastics and fabrics. This offers the prospect of developing a range of energy harvesting devices which can access large mechanical deformations of these flexible substrates for conversion to electrical energy. We have developed piezoelectric energy harvesters based on ZnO nanorod p-n junctions on flexible substrates, using the p-type conducting polymer PEDOT:PSS to coat the nanorod tips, acting both as a top contact surface and reducing the screening effect that can limit the efficiency of ZnO-based devices. Furthermore, by coating the nanorods with the p-type semiconductor CuSCN the internal carrier density can be reduced, leading to a significant increase in power output. The mechanisms underlying these effects will be discussed, and the importance of thorough characterisation and testing of the devices will be highlighted. This has demonstrated that despite relatively low voltage output from these devices (up to 1 V), the low internal impedance (~10 kOhm) can lead to higher power output than equivalent devices incorporating insulating layers to limit screening. We are investigating the application of these devices to remote sensor nodes for helicopter health monitoring, and the potential benefits, challenges and key considerations of this application will be discussed.

15:30 A review on Advances in Thin Film Nanotechnology and Nanofabrication of Smart Multifunctional Metal Insulating Transition Oxide Heterostructures for Next Generation Femtosecond Optoelectronic Sensors and Nanodevices **X.I.5**

Authors : Mohamed Saad
Affiliations : Queen's University Belfast

Resume : Abstract Smart multifunctional complex oxide heterostructures such as the metal insulating transition (MIT) thin films and nanoparticles have recently received a renewed attention due to their promising novel nanotechnological applications and breakthrough in switching, sensing, energy-efficient buildings and non-volatile memories. There are several factors, which make this review and talk particularly timely and important. Firstly, there is a market pressure, primarily from the nanoelectronic industry and energy sector to develop novel devices at low cost. Secondly, there is opportunity for novel exploration, new functionality and breakthrough due to the recent developments in thin film growth nanotechnology and nanocharacterisation techniques. Thirdly, there is a lack of information on Health and Safety issues concerning the MIT nanoparticles fabrication including their negative impact on environment. This feature review attempts to discuss the thin film growth nanotechnology and nanofabrication techniques including process optimisation of the MIT oxides. In particular, the evolution of thin film and nanoparticles fabrication techniques using PLD, MBE, CVD, LPCVD, PECVD, MOCVD, ALD, FIB and Sputtering systems

are critically reviewed. Emerging applications and multifunctional nanocharacterisation techniques of these smart complex oxides are also covered.

16:00 *Coffee break*

Poster Session I: Materials for Environmental Sensing and Devices : Michele Penza and Albert Romano-Rodriguez

16:30 **Easy low temperature green route to crystalline ZnO nanostructures for H2S sensing** **X.PI.1**

Authors : Stefano Diodati,a Jörg Hennemann, b,c Bernd Smarsly, b and Silvia Grossa, a,d*
Affiliations : Stefano Diodati, Dipartimento di Scienze Chimiche, Università degli Studi di Padova, via Marzolo 1, 35131- Padova; Jörg Hennemann, Physikalisch-Chemisches Institut, Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 58, 35392 Giessen, Germany; Bernd Smarsly, Physikalisch-Chemisches Institut, Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 58, 35392 Giessen, Germany; Silvia Gross, Istituto per l'Energetica e le Interfasi, IENI-CNR, Dipartimento di Scienze Chimiche, Università degli Studi di Padova, via Marzolo 1, 35131- Padova and INSTM, UdR di Padova, Italy;

Resume : Crystalline nanosized ZnO was synthesized at 135°C through a wet chemistry route combining coprecipitation of oxalates and subcritical hydrothermal treatment. The resulting materials were characterised from a compositional (XPS, ICP-MS), morphological (SEM, TEM) and structural (powder XRD, SAED) point of view. The obtained nanostructured ZnO was employed in H2S sensing, taking advantage of the change in conductance upon reaction with H2S. When exposed to 5 ppm H2S at 150°C, the sensor conductance increased by more than two orders of magnitude, with near-linear rate over time. This behaviour is typical of a gas dosimeter [1] and suggests progressive conversion of ZnO to ZnS with exposure to H2S. Often such accumulation is unwanted,since usually reaching a certain conductance value is proportional to the gas concentration to be determined; in our case, the signal increases until saturation is reached, which is advantageous, as through the accumulation it is possible to detect very low gas concentrations. Tests carried out at 450°C showed that different gas concentrations caused the sensor conductivity to increase with different constant slopes, and that conductivity rapidly returned to the starting value once the gas flow was removed, implying that sensor regeneration took place. Scanning electron microscopy collected on the ZnO samples before use and after regeneration at 450°C showed no changes in the material morphology although full regeneration to ZnO was achieved. [1] Marr et al., J. Sens. Sens. Syst. 2014, 3, 29

16:30 **Synthesis, structural characterization, and UV-enhanced gas-sensing properties of ZnO-SnO2 heterojunctions** **X.PI.2**

Authors : Luís F. da Silva, Ariadne C. Catto, Osmando F. Lopes, Khalifa Aguir, Valmor. R. Mastelaro, Caue Ribeiro, and Elson Longo
Affiliations : LIEC, Institute of Chemistry, São Paulo State University, Araraquara, São Paulo, Brazil; Instituto de Física de São Carlos, Universidade de São Paulo, São Carlos, São Paulo, Brazil; EMBRAPA Instrumentação, São Carlos, São Paulo, Brazil; Université Aix-Marseille, Faculté St Jerôme, Marseille, France.

Resume : Gas detection is important for controlling industrial, and vehicle emissions, agricultural residues, and environmental control. In last decades, several semiconducting oxides have been used to detect dangerous or toxic gases. The excellent gas-sensing performance of these devices have been observed at high temperatures (~250oC), which forbids the use for the detection of flammable and explosive gases. In this way, ultraviolet light activated gas sensors have been a simple and promising alternative to achieve room temperature sensitivity. Among the semiconductor oxides which exhibit a good performance as gas sensor, the zinc oxide (ZnO) and tin oxide (SnO2) have been highlighted. Nevertheless, their poor selectivity is the main disadvantage for application as gas sensor devices. Recently, heterostructures combining these two semiconductors (ZnO-SnO2) have been studied as an alternative way to enhance the gas sensor performance (sensitivity, selectivity, and stability). In this work, we investigated the influence of mass ratio Zn:Sn on the properties of ZnO-SnO2 nanocomposites prepared by hydrothermal treatment for 4 hours at 200oC. The crystalline phase, surface, and morphological features were characterized by X-ray diffraction (XRD), high-resolution transmission electron (HR-TEM), and X-ray photoelectron spectroscopy (XPS) measurements. The gas sensor measurements were carried out at room-temperature under ultraviolet (UV) light irradiation using different ozone levels (0.06 to 0.61 ppm). The XRD measurements indicate the presence of ZnO and SnO2 crystalline phases, without the evidence of solid solution formation. HR-TEM analysis revealed that a good contact between the SnO2 nanoparticles and the ZnO nanorods, which are very important since interface characteristics between nanostructures is considered a challenge to development new and efficient heterostructures. Electrical measurements proved that the best ozone gas-sensing performance is obtained for ZnO:SnO2 (50:50) nanocomposite under UV light irradiation. Its sensitivity was around 6 times higher when compared to SnO2 pure, a traditional ozone gas sensor. These results demonstrate the potential of ZnO-SnO2 heterojunctions for the detection of ozone gas at room-temperature when irradiated with UV light irradiation.

16:30 Local structure and gas-sensing properties of the nanocrystalline Zn1-xCoxO films **X.PI.3**

Authors : Ariadne C. Catto, Luis F. da Silva, Khalifa Aguir, Valmor Roberto Mastelaro
Affiliations : Univ de São Paulo, São Carlos, Brazil; Institute of Chemistry, São Paulo State University, Araraquara, Brazil; Université Aix-Marseille, Faculté St Jerôme, Marseille, France; Univ de São Paulo, São Carlos, Brazil;

Resume : Zinc oxide (ZnO) pure or doped are one of the most promising metal oxide semiconductors for gas sensing applications due the well-known high surface-to-volume area and surface conductivity. It was show that ZnO is an excellent gas-sensing material for different gases such as CO, O2, NO2 and ethanol. In this context, pure and doped ZnO exhibiting different morphologies and a high surface/volume ratio can be a good option regarding the limitations of the current commercial sensors. Different studies showed that the sensitivity of metal-doped ZnO (e.g. Co, Fe, Mn,) enhanced its gas sensing properties. Motivated by these considerations, the aim of this study consisted on the investigation of the role of Co ions on structural, morphological and the gas sensing properties of nanostructured ZnO samples. ZnO and Zn1-xCoxO (0 < x < 5 wt%) thin films were obtained via the polymeric precursor method. The sensitivity, selectivity, response time and long-term stability gas sensing properties were investigate when the sample was exposed to different

concentration range of ozone (O3) at different working temperatures. The gas sensing property was probed by electrical resistance measurements. The long and short-range order structure around Zn and Co atoms were investigate by X-ray diffraction and X-ray absorption spectroscopy. X-ray photoelectron spectroscopy measurement were performed in order to identify the elements present on the film surface as well as to determine the sample composition. Microstructural characteristics of the films were analyzed by a field-emission scanning electron microscope (FE-SEM). Zn1-xCoxO XRD patterns were indexed to the wurtzite ZnO structure and any second phase was observed even at a higher cobalt content. Co-K edge XANES spectra revealed the predominance of Co2+ ions. XPS characterization revealed that Co-doped ZnO samples possessed a higher percentage of oxygen vacancies than the ZnO samples, which also contributed to their excellent gas sensing performance. Gas sensor measurements pointed out that ZnO and Co-doped ZnO samples exhibit a good gas sensing performance concerning the reproducibility and a fast response time (around 10 s). Furthermore, the Co addition contributed to reduce the working temperature for ozone detection and improve the selective sensing properties.

16:30 SiNWs for crude oil Polycyclic Aromatic Hydrocarbon (PAH) detection **X.PI.4**

Authors : N. Nafie, M. Bouaïcha
Affiliations : Laboratoire de Photovoltaïque, Centre de Recherches et des Technologies de l'Energie, Technopole de Borj-Cédria, BP 95, Hammam-Lif, 2050 Tunis, Tunisia

Resume : Due to their high surface/volume ratio, silicon nanowires (SiNWs) could be very suitable nanostructures for gas sensing applications. In this work, SiNWs is used for crude oil Polycyclic Aromatic Hydrocarbon (PAH) detection. The structure of the fabricated device is Al/SiNWs/c-Si/SiNWs/Al. For PAH detection, we performed adequate experimental setup to measure variation of the serial resistance Rs during different adsorption/desorption cycles of the device. As a result, we found that for high PAH contamination dose, the device doesn't exhibit reproducible behavior after contaminant flushing. However, when the device is heated during nitrogen flushing, we found that for concentration of several thousands of ppm, a complete desorption of PAH molecules occurs leading to identical adsorption/desorption cycles but shifted to high Rs values. Effects of the amount of PAH contaminant and the heating temperature of the device are also discussed.

16:30 Tailoring the UV Photoresponse of ZnO Nanowire FETs for Environmental Monitoring **X.PI.5**

Authors : Ming-Pei Lu, Chieh-Wei Chen, Ming-Yen Lu,
Affiliations : National Nano Device Laboratories, National Applied Research Laboratories, Hsinchu 300, Taiwan; Graduate Institute of Opto-Mechatronics, National Chung Cheng University, Chia-Yi 62102, Taiwan;

Resume : In this report, we used the oxygen plasma treatment technique to modify the density of oxygen-related defect states in ZnO nanowires (NWs) for tuning the UV response characteristics. After the oxygen plasma treatments, we utilized the XPS measurement to confirm the reduction of the defect density of oxygen vacancy. The defect densities of as-grown and oxygen plasma-treated NW FETs were investigated by using the low-frequency noise analysis method, revealing that the surface defect density of NW FETs

can be reduced by using the oxygen plasma treatment. As a result, the donor concentration of NWs was decreased with increasing the exposure time of oxygen plasma treatment. We also found that the UV response and recovery times of NW FETs can be tailored through the oxygen plasma treatment. The physical mechanism behind the effect of oxygen plasma treatment on photoresponse of NWs was discussed. This report can pave a way toward the development of nanoscale FET photodetectors of hazardous UV light for the environmental monitoring applications.

16:30 Studies analytical for the detection of glucose based carbon nanotube **X.PI.7**

Authors : O.Zeggai (1.2) , A.Ould-abbes (1) , M. Belarbi (1), N. Sahouane (1), H. Zeggai (1), N-E. Chabane-Sari (1).
Affiliations : (1) Research Unit of Materials and Renewable Energies (URMER), Abou Bakr Belkaïd University, B.P. 119, Tlemcen, Algeria (2) Hassiba ben bouali university, BP 151,02000 chlef

Resume : In recent years, a new form of carbon nanotube electrode spread like promising nanoelectronic devices based on carbon and for biological and medical applications. Because of their physical property, chemical and electrical. Carbon nanotubes can be effectively used as electrochemical sensors. The integration of carbon nanotubes provides a good solid support for the immobilization of enzymes. Determining glucose levels using biosensors, especially in medical diagnostics and in food industries. This action provides high accuracy and rapid detection rate. The purpose of this study includes the presentation of the transistor-based biosensor field effect structure with a grid of carbon nanotubes for detection of glucose with an analytical study of biosensor, and in this model we present a relationship combines between the glucose concentration and one of transistor parameters. .

16:30 In-situ study of sensor response in copper oxide materials **X.PI.8**

Authors : Marcelo Ornaghi Orlandi*(1), Diogo Paschoalini Volanti(2), Anderson André Felix(1), Pedro Henrique Suman(1), José Arana Varela(1)
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Resume : In this work we report an advanced study of gas sensor performance of copper oxide (CuO) urchin-like structures synthesized by microwave assisted hydrothermal method. Copper oxide in an interesting p-type semiconductor and literature shows that it can present high sensitivity to hydrogen (H2) with good selectivity. In order to study the mechanisms related to the sensor response of CuO structures, we developed a special sample holder which enables the simultaneous characterization of materials by X-ray absorption near edge structure (XANES) and electrical measurements. XANES measurements allowed to know the local structure and the oxidation state of the material while electrical measurement monitored the sensor signal of material. We studied the material response in synthetic air and pure nitrogen (N2) baselines under H2 analyte exposure. Quantitative XANES analyses showed that the CuO material can have its surface completely reduced when exposed to H2 in N2 baseline and electrical measurements confirm the abrupt decrease in the material resistance. This superficial reduction is reversible after exposition of sample to a

synthetic air atmosphere. Morphological studies were conducted by scanning electron microcopy (SEM) and showed that materials had morphological changes after the reducing and re-oxidation processes. So, sensor response models for CuO material based on these findings were proposed.

16:30 GRAPHENE/TITANIUM (IV) OXIDE NANOCOMPOSITE - BASED HYPOXANTHINE SENSOR FOR ASSESSMENT OF MEAT FRESHNESS **X.PI.9**

Authors : Jasmine A.V. Albelda (1,2,3), Aytekin Uzunoglu (1), Gil Nonato C. Santos (2), Lia A. Stanciu (1)
Affiliations : (1)School of Materials Engineering, Purdue University, 701 West Stadium Avenue, West Lafayette, IN 47907, USA; (2)Physics Department, De La Salle University, 2401 Taft Avenue Manila, Philippines 1004; (3) Philippine Normal University, Taft Avenue Manila, Philippines 1000

Resume : We report on the fabrication of a graphene/titanium dioxide nanocomposite (Gr/TiO2) and its use as an effective electrode material in an amperometric hypoxanthine sensor for meat freshness evaluation. The nanocomposite was characterized by TEM, XRD, FTIR, TGA, BET, and CV using the redox couples [Fe(CN)6]-3/-4 and [Ru(NH3)6] 3/ 2 respectively. The Gr/TiO2 nanocomposite offered a favorable microenvironment for direct electrochemistry of xanthine oxidase (XOD). The fabricated Nafion-XOD-Gr/TiO2 sensor exhibited excellent electro catalytic activity towards hypoxanthine with linear range of 20 µM to 512 µM, limit of detection (LOD) of 9.5 µM, and sensitivity of 4.1 nA/µM. In addition, the biosensor also demonstrated strong anti-interference properties in the presence of uric acid, ascorbic acid and glucose. Minimal interference of xanthine was observed at ~7%. Moreover, the biosensor showed good repeatability (4.3% RSD) and reproducibility (3.8% RSD). The reported biosensor was tested towards the detection of hypoxanthine in pork tenderloins stored at room temperature for seven days. There was a good correlation between biosensor response and measurements obtained by a standard enzymatic colorimetric method (r = 0.9795). The Gr/TiO2 nanocomposite is therefore an effective electrode material to be used in electrochemical biosensors to assess the freshness of meat.

16:30 Study of conducting mixture of Carbon nanotubes/Polyaniline for development of a NH3, CO2, and CO selective gas sensor **X.PI.10**

Authors : Stefan Ionut SPIRIDON (1), Eusebiu Ilarian IONETE (1), Bogdan Florian MONEA (1), Ioan STAMATIN (2), Ana-Maria IORDACHE (2)
Affiliations : (1) National R&D Institute for Cryogenics and Isotopic Technologies – ICIT Rm.Valcea, Uzinei Str. RM Valcea, No. 4, 240050, Valcea, Romania. (2) University of Bucharest. Faculty of Physics, 3Nano-SAE Research Center, P.O. Box MG-38, 077125, Magurele, Romania.

Resume : Electrical conductivity change can be used to detect different chemical species by sensors with active layer composed of an electrically conducting polymer formed from a mixture of carbon nanotubes (CNT) and polyaniline (PANi). Depending on the doping level, estimated by relative carbon content, the electrical conductivity of PANi could be improved by orders of magnitude. Composite mixture characterized by high electrochemical activity and improved stability, with different gas selectivity mechanisms could be a solution for an efficient low-powered sensor-system. This paper presents

an NH3, CO2, and CO selective gas sensor unit with practical application in the field of environmental monitoring, healthcare, automation, industrial process control, etc. Disseminated basic research will describe the sensing mechanism of the sensor and also the selectivity criteria for gas interaction.

16:30 Gas sensors based on sulfonated single walled carbon nanotubes **X.PI.11**

Authors : Ionete Eusebiu Ilarian (1) Stefan Ionut Spiridon (1) Bogdan Florian Monea (1) Daniela Ion Ebrasu (1) Ioan Stamatin (2)
Affiliations : (1) National R&D Institute for Cryogenics and Isotopic Technologies – ICIT Rm.Valcea,POBox 7, 4 Uzinei Str. RM Valcea, 240050, Valcea, Romania. (2) University of Bucharest. Faculty of Physics, 3Nano-SAE Research Center, P.O. Box MG-38, 077125, Magurele, Romania.

Resume : In this work, sulfonated single walled carbon nanotubes (SWCNTs) were used as sensing substrate for different gases detection. To synthesize sulfonated SWCNT the SWCNTs were treated with sulfuric acid, under different working conditions, at temperatures ranging from 60°C to 300°C, and further characterized by Scanning electron microscopy (SEM), Fourier transform infrared spectroscopy (FT-IR) and Raman spectroscopy. The obtained solutions were deposited as sensible material on an interdigitized electrode structure and used as gas sensors for the detection of CO, NO, NH3 and CH4, respectively. The response and the recovery time of the build sensors structures having sulfonated CNTs as support were presented and compared. Furthermore, several important parameters controlling the fabrication of the sensible substrates were investigated and optimized. Overall it was concluded that the sulfonated single walled carbon nanotubes are very good candidates for SWCNTs based gas sensors.

16:30 Very low temperature cryogenic sensor with single walled carbon nanotubes **X.PI.12**

Authors : Bogdan Florian MONEA, Eusebiu Ilarian IONETE, Stefan Ionut SPIRIDON, Amalia SOARE, Alexandru RIZOIU
Affiliations : National R&D Institute for Cryogenics and Isotopic Technologies – ICIT Rm.Valcea, Uzinei Str., No.4, Rm. Valcea, 240050, Valcea, Romania

Resume : The present study explores the possibility of using single walled carbon nanotubes as sensible elements for a very low temperature cryogenic sensor, 2K - 77K. The superior material properties of carbon nanotubes (CNTs) have suggested that it is possible to create a device that will meet these requirements and also have better performance when compared to devices currently available in the market. A resistive structure was designed and carbon nanotubes, dropcasted from a solution, were aligned by dielectrophoretic method between structure electrodes. The assembly formed together with a reference sensor where connected to an acquisition system, by a 4-points method, and where subjected to resistance measurement, in cryogenic field, down to 2K. The resulting device exploits the extremely small size of SWCNTs as well as their superior thermal and electrical properties by deriving the temperature based on a change in electrical resistance. From the dependence of electrical resistance versus temperature it can be concluded that the approach presents a series of advantages and can be employed in the fabrication procedure of a microsensor for cryogenic applications.

16:30

Preparation and SERS investigation of ordered arrays of Au nanotubes

X.PI.13

Authors : Yonghui Chen, Jinglai Duan, Khan Maaz and Jie Liu.
Affiliations : Institute of Modern Physics, Chinese Academy of Sciences.

Resume : Ordered arrays of Au nanotubes, with an external diameter of 150 nm, length of 1.2±0.3 μm and wall thickness of 15±5 nm, were successfully fabricated in porous polycarbonate (PC) ion-track templates by electrochemical deposition. The morphologies and crystal structure of the nanotubes were characterized by scanning electron microscopy (SEM), transmission electron microscopy (TEM) and X-ray diffraction (XRD). The extinction spectra and electric field distributions of Au nanotube were investigated theoretically by finite difference time-domain (FDTD) method. It was shown that, at the main plasmon peak wavelength, Au nanotube possesses highly strong electric field distributions around both inside and outside surfaces, which demonstrated that such nanotubes could be a new and interesting candidate to be used as surface enhanced Raman scattering (SERS) substrate. Moreover, this nanotube-based substrate can be utilized as a sensor for the environmental monitoring and food safety inspection. The expected high SERS activity was confirmed by Raman spectra of 4-Mercaptopyridine (as a probe molecule) adsorbed onto Au nanotube substrate. In addition, the SERS spectra of the bulk standard activated Au substrate were also measured in this work.

16:30

Influence of the electropolymerization conditions on the sensing properities of Polypyrrol/AuNP composites towards phenols

X.PI.14

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Resume : Polypyrrole (Ppy) is one of the most extensively studied conducting polymers due to its good electrical conductivity and redox properties [1]. Ppy films can be easily generated by electropolymerization as a strong adherent layer using different electrochemical techniques [2]. Electrodes chemically modified with Ppy have a good electrocatalytic activity. The structure and sensing properties of the Ppy films are considerably influenced by the electrochemical method used for the polymerization (potentiostatic, galvanostatic or potentiodynamic), by the electrochemical conditions (voltage, intensity, scan rate, etc.), and by the other experimental conditions such as the nature and concentration of the doping agent or the nature of the substrate [3]. Recently, composite nanomaterials based on conducting polymers and metal nanoparticles (NPs) have been developed. Gold nanoparticles (AuNPs) have attracted considerable interest because of their unique optical, electronic and catalytic properties [4]. Conducting PPy/AuNP composites exhibit improved physical and chemical properties over their single-component counterparts and are the focus of intensive research. Ppy/AuNP composites can be prepared by chemical and electrochemical polymerization. Electrochemical methods provide a better control of the structure and properties of the composite by controlling the electrochemical conditions during film generation [5]. It could be expected that the electrocatalytic and the sensing properties of the Ppy/AuNPs films directly depend on the polymerization conditions. One of the fields where electrochemical sensors are having an important success is

in the detection of phenolic compounds, which are important pollutants in waters [6]. As phenols are electroactive compounds, they can be detected by amperometric or voltammetric techniques using a great variety of electrodes. Ppy/AuNPs composites could be good candidates as electrocatalytic materials for the detection of phenols. The objective of this work was to develop new voltammetric sensors based on electrodeposited Ppy/AuNPs for the detection of catechol (an antioxidant of interest in the food industry) and to evaluate the influence of the electrodeposition method in their performance. For this purpose Ppy/AuNP films doped with 1-decanesulfonic acid (DSA) were deposited using different methods. The first approach consisted on the electrodeposition of the Ppy/AuNPs films from a solution containing the monomer and the trichloroauric acid (cogeneration method). The second approach consisted of the electrodeposition of the Ppy/AuNPs composited from a solution containing the monomer and gold nanoparticles previously formed (trapping method). In both methods, electrodeposition was carried out by chronoamperometry (CA) and by chronopotentiometry (CP). Particular attention was paid to the study of the influence of the substrate used for the electrodeposition that was carried out onto classical platinum electrodes and on stainless steel substrates. This aspect could play a crucial role not only in the structure, properties and performance of the sensor but also in the final price. Using CA, the polymerization charge was strongly dependent on the presence of AuNPs and the mass deposited in the absence of AuNPs was higher than the mass deposited in the presence of gold. The charge calculated for films obtained by cogeneration was superior than by trapping. That is, the amount of polymer deposited followed the same trend whatever CP or CA were used. This result also points to the role of AuNPs in the nucleation of Ppy, difficulting the oxidation of the monomers. Scanning electron microscopy (SEM) demonstrated that in all cases gold nanoparticles of similar size (30-40 nm) were uniformly dispersed in the Ppy matrix. The amount of AuNPs incorporated in the Ppy films was higher when electropolymerization was carried out by CP. Besides, cogeneration method allowed for the incorporation of a higher number of AuNPs than trapping. Electrochemical Impedance Spectroscopy (EIS) experiments demonstrated that the insertion of AuNPs modified the electrical behavior and increased the conductivity. The cogeneration method combined with chronopotentiometry seemed to be the most suitable electrodeposition technique to prepare electrochemical sensors.experiments demonstrated that the insertion of AuNPs increased the conductivity. The electrocatalytic and sensing properties towards catechol of Ppy/AuNP electrodes were analyzed. Catechol produced the expected well-shaped redox pair generated by the two-electron oxidation/reduction of the orto-dihydroquinone to benzoquinone. The reversibility of the peaks was improved with the incorporation of the AuNPs and the intensity of the peaks increased with the concentration of AuNPs. These effects were stronger in films deposited by CP than in films deposited by CA, due to the higher concentration of nanoparticles. In contrast, the method to insert the nanoparticles (trapping or cogeneration) only produced small changes in the intensities and positions of the peaks, probably due to the minimal differences in the AuNPs concentration. The electrocatalytic effect was stronger in films deposited on platinum than in SS. The limits of detection (LOD) were in the range from 10−5 to 10−6 mol/L. LODs attained using films deposited on platinum were lower due to a synergy between AuNPs and platinum that facilitates the electron transfer, improving the electrocatalytic properties. Such synergistic effects are not so pronounced on stainless steel, but acceptable LODs are attained with lower price sensors. References [1] Ramanavicius, A.; Ramanaviciene, A; Malinauskas, A. Electrochim. Acta, 51 (2006) 6025. [2] Li,

C.M.; Sun, C.Q.; Chen, W.; Pan, L. Surf. Coat. Tech. 198 (2005) 474. [3] Chillawar, R.R.; Tadi, K.K.; Motghare, R.V. J. Anal. Chem. 70 (2015) 399. [4] Yoon, H. Nanomaterials 3 (2013) 524. [5] Rapecki, T.; Donten, M.; Stojek, Z. Electrochem. Commun. 12 (2010) 624. [6] Hurtado E.; Gomez, M.; Carrasco, A.; Fernandez, A. J. Pharm. Biomed. Anal. 53 (2010) 1130.

16:30

Ultra-High Sensitive Hydrogen Sensors Based on Pd-coated wet-etched n- and p-type Si Nanowires

X.PI.15

Authors : Jisun Baek?, Byungjin Jang?, Jeongmin Kim?, Sera Shin ?, Taeyoon Lee? and Wooyoung Lee*?
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Resume : Here we report the hydrogen (H2) sensing properties in Pd-coated vertical Si nanowire (NW) arrays fabricated by wet chemical etching of n- and p-type Si wafers. Pd was deposited on the top surface of dense wet-etched vertical Si NW arrays with an average height of 30 ?m using an ultra-high vacuum DC magnetron sputtering system.In case of n-type H2 sensors, the sensing properties of sensitivity, response time, and detection limit were found to be 94 % (1 % H2), 31 s and 5 ppm, respectively in air. Also, the sensing properties in p-type H2 sensors were shown to be 1700 % (1 % H2), 9 s, 5 ppm, respectively. Our results indicate that the sensing properties in the p-type sensors are much better than that in the n-type sensors. In-situ Hall measurements showed that the carrier concentrations in the n- and p-type sensors are 6.4×10^18 and 6.3×10^19 in air and 7.1×10^18 and 5.8×10^18 in 10 % H2, respectively. We found that the change of the carrier concentrations in the p-type sensors (10 times) is much larger than that in the n-type sensors (1.2 times) before and after exposed to H2. The results are due to the change of the contacts at PdH/Si interface, depending on the major carrier type of Si; the Schottky to Ohmic contact for n-type Si and Ohmic to Schottky contact for p-type Si. The H2 sensors are also found to detect dissolved H2 gas in oil.

16:30

Al-Doped ZnO Nanoparticles for the Detection of 2-CEES As a Simulant of a Mustard Gas

X.PI.16

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Resume : The sensing behaviors as a function of temperature and gas concentration in Al ZnO nanoparticles have been investigated for the detection of 2-CEES (2-choloro ethyl ethyl sulphide) as a simulant of mustard gas. In order to study the effect of doping on the sensing properties, ZnO nanoparticles were doped with Al ions as mixing with a solution contains Al acetate using a hydrothermal method. The ZnO nanoparticles were dispersed by a dropping method on the interdigitated Pt electrode using ?-terpineol paste. The average sizes of the Al undoped- and doped- ZnO nanoparticles are ~40 nm and ~25 nm, respectively. The sensing properties of the Al-doped ZnO based 2-CEES sensors were measured via real-time monitoring of electrical resistance change upon exposure of 2-CEES gas in air. The responses (Ra-Rg/Rg) (Ra: R in air; Rg: R in 2-CEES) of the sensors based on Al undoped- and doped-ZnO nanoparticles were measured to be 110 and 197, respectively, in 5 ppm 2-CEES. Also, the response times of the sensors were found to

be 7.6 s and 2 s, respectively. The enhanced sensing properties in the Al-doped ZnO nanoparticles are attributed to the higher surface area to volume ratio and the increase of oxygen vacancies. We demonstrate that the 2-CEES sensors based on Al undoped- and doped- ZnO nanoparticles show excellent sensing properties such as response, response time, superior to the sensing properties in the literatures [1]. [1] L.A. Patil ,etal, Sens. Actu. B, 160 (2011) 234.

16:30 Detection of pollutant gases by nanostructured cobalt ferrite **X.PI.17**

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Resume : The reactivity and sensitivity of the sensing materials can be tailored by controlling their composition, structure, phase, shape, size, and size distribution. In particular, the detection function of a sensing material is dependent of the exposed crystallographic facets. Hence, we synthesized cobalt ferrites as nanoparticles with various shapes and sizes, as well as thin films, for the monitoring of low level of pollutant gases in air. Cobalt ferrite proved to be an interesting material due to its good chemical stability, magnetic behavior and catalytic activity [1-2].The detection of low concentrations of NO2 by CoFe2O4 nanooctahedra and by nanostructured thin films was studied. Octahedron-like nanoparticles of CoFe2O4 were synthesised using a hydrothermal technique [3]. Thin films were obtained by spin coating from a solution of iron and cobalt acetylacetonate precursors. The nanostructures were characterized by several microscopy techniques. CoFe2O4 nanooctahedra exhibit a high sensibility to 10 ppm NO2, at 200°C and the shape effect on sensibility was clearly demonstrated. Thin films with high amount of cobalt (Co1.8Fe1.2O4) showed a p type response and enhanced sensitivity compared to the n type response of CoFe2O4. [1] L. Ajroudi,S. Villain,V. Madigou,N. Mliki,Ch. Leroux, J. Cryst. Growth 312 (2010) 2465–2471. [2] L. Ajroudi, V. Madigou, S.Villain, L. Bessais, N. Mliki, Ch. Leroux, Materials Research Bul., 59, 49-58, 2014. [3] A. L. Lopes-Moriyama, V. Madigou, C. Pereira de Souza, Ch. Leroux, Powder Tech., 256,482-489 , 2014.
Acknowledgments: This work was done in the general framework of the CAPES COFECUB Ph-C 777-13 french – brazilian cooperation project.

16:30 Sensitive detection of hydrocarbon gases using electrochemically Pd-doped ZnO-based chemiresistors **X.PI.18**

Authors : Elena Dilonardo,1,2 Michele Penza,3 Marco Alvisi,3 Gennaro Cassano,3 Cinzia Di Franco,4 Francesco Palmisano,1 Luisa Torsi,1 Nicola Cioffi1
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Resume : ZnO nanorods, prepared by hydrothermal sol-gel synthesis with further annealing at 550°C,[1] and Pd-decorated ZnO nanorods, prepared by a direct electrochemical decoration of hydrothermal ZnO

nanostructures by Pd NPs,[2] and subsequently subjected to stabilization at 550°C, were proposed as active layer in chemiresistive sensors for pollutant gas detection (e.g. NO2, C4H10). The effect of the presence of the metal catalyst on the ZnO-based sensor performance (e.g., sensitivity and selectivity) were analyzed, comparing the sensing results with those of undoped ZnO nanostructures. In particular, the gas sensing properties of pristine and Pd-functionalized ZnO nanorods were studied at an operating temperature of 300°C for a wide range of target gas concentrations. Specifically, for the detection of NO2 gas, pristine ZnO nanordos showed the highest selectivity and sensitivity; instead, Pd-doped ZnO nanorods revealed a higher sensitivity and selectivity towards hydrocarbon gases, such as CH4, and C4H10, comparing to those reported for the undoped ZnO-based gas sensor. Finally, the sensing mechanisms of pristine and Pd-doped ZnO nanorods towards the analyzed gaseous pollutants have been proposed, considering the effect of their chemical composition and morphology evaluated by XPS and SEM analyses, respectively. [1] E. Dilonardo et al., Beilstein J. Nanotechnol. 2016, 7, 22. [2] M.T. Reetz et al., J. Am. Chem. Soc. 1994, 116, 7401.

16:30

SERS Using Gold Nanoparticles at Liquid-Liquid Interfaces

X.PI.19

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Affiliations : Imperial College London

Resume : The project concerns self-assembly of gold nanoparticles at the water-oil interface. Through modification of the liquid-liquid interface (LLI) system, certain target molecules are expected to be detected at ultralow concentrations (aiming at the nanomolar range). A range of LLI systems will be tested, including different sizes of gold NPs, the functionalisation of the NPs, different Raman reporter molecules, etc. The target molecule is determined to be heavy metal ions at this stage.[1] The behaviour of the system is characterised by SEM, TEM, UV-Vis and surface enhanced Raman spectroscopy (SERS). The limit of detection (LOD) of the system is mainly determined by SERS through the presence and the intensity of characteristic peaks. Results of this LLI system can be compared with other systems to see its advantages in terms of signal enhancement and LOD, complexity of preparation techniques, etc. 1. M. P. Cecchini, V. A. Turek, A. Demetriadou, G. Britovsek, T. Welton, A. A. Kornyshev, J. D. E. T. Wilton-Ely and J. B. Edel, Advanced Optical Materials, 2014, 2, 966-977

16:30

ADSORPTION OF PARA-NITROPHENOL ON CYCLODEXTRIN BASED-MATERIAL COATED BY BENTONITE

X.PI.20

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Resume : SORPTION OF P-NITROPHENOL FROM WATER BY BENTONITE/ POLY(4-VINYLPYRIDINE-G-(6-O-MONOTOSYL-6-DESOXY-B-CYCLODEXTRIN)) COMPOSITE WAS STUDIED. STUDIES CONCERNING THE SORPTION KINETIC AND ISOTHERM ARE PRESENTED AND DISCUSSED. RESULTS OF ADSORPTION EXPERIMENTS SHOWED THAT THE ADSORBENT EXHIBITED HIGH SORPTION CAPACITIES TOWARD P-NITROPHENOL. THE ADSORPTION CAPACITY OF THE BENTONITE/ POLY(4-

VINYLPYRIDINE-G-(6-O-MONOTOSYL-6-DESOXY-B-CYCLODEXTRIN)) MATERIAL INCREASED AS THE DOSAGE OF THE MATERIAL INCREASED. TWO ISOTHERM EQUATIONS HAVE BEEN TESTED IN THE PRESENT STUDY, NAMELY FREUNDLICH AND LANGMUIR. THE CHARACTERISTIC PARAMETERS FOR EACH ISOTHERM HAVE BEEN DETERMINED. THE FREUNDLICH EQUATION REPRESENTED THE BEST FIT OF EXPERIMENTAL DATA THAN THE OTHER ISOTHERM EQUATION.

16:30 Determination of Nonylphenol and Pentachlorophenol at an Electrode Modified with a ZnS/g-C3N4 /DNA Nanocomposites Film **X.PI.21**

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Affiliations : Jing Zou

Resume : ZnS quantum dots (QDs) were prepared by solvothermal method, and ZnSQDs/g-C3N4 /DNA nanocomposites were preprated with ZnSQDs, DNA and g-C3N4 by stir-mixing method. The glassy carbon electrode(GCE) was modified with ZnSQDs/g-C3N4/DNA nanocomposites by polymerization. The effects of pH, amount of electrocatalyst and modification method were researched. The novel electrochemical sensors of environmental hormones were built, and the electrochemical behaviors of nonylphenol and pentachlorophenol at the modified electrode were investigated by cyclic voltammetry and differential pulse voltammetry. The experimental results showed that the modified electrode had a significant electrocatalytic activity for nonylphenol and pentachlorophenol. Under the optimized experimental conditions, the linear ranges and the detection limits of nonylphenol and pentachlorophenol are 0.01μM ~ 20μM, 0.01μM ~ 10μM, 3.3 ×10-9 M, and 3.3×10-9 M, respectively. Nonylphenol and pentachlorophenol in Lake were determinated with ZnSQDs/g-C3N4/DNA/GCE by differential pulse voltammetry. Their methodology recoveries were higher than 90%.

16:30 Effects of violet-, green-, and red-laser illumination on gas-sensing properties of SnO thin film **X.PI.22**

Authors : Vu Xuan Hien(1), Kwang-Min Jo(2), Sangwook Lee(2), Joon-Hyung Lee(2), Jeong-Joo Kim(2), Young-Woo Heo(2)*
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Resume : The light-induced or light-activated gas-sensing properties of a sensor may offer many advantages, including the ability to operate with greater stability and reduced power consumption or at room temperature to prevent unwanted reactions of combustible gases. Initial studies have primarily been carried out using SnO2 , In2O3, ZnO, TiO2, and SnO2-core/ZnO-shell, with activation by ultraviolet (UV) light because its energy is equal to or larger than the bandgaps of these materials. Although visible-light irradiation can be applied to some n-type semiconductors such as ZnO or WO3, a two-photon or multi-photon excitation process, electron excitation from an intragap band [9], or lower-bandgap materials such as p-type metal-oxide semiconductors are preferred for investigations on visible-light-induced gas-sensing properties. We examined the gas-sensing properties of a 10-nm-thick SnO thin film under the illumination of violet, green, and red laser beams at room temperature. A comparison of the gas-sensing outputs of the device after operation in the dark at elevated temperatures (100, 150,

and 200°C) and when illuminated by a laser beam at room temperature indicated that this metal-oxide film had good gas-sensing performance and excellent stability under the illumination of the violet beam. When exposed to several target gases, including NO2, SO2, H2S, and NH3, the SnO thin film was most sensitive to H2S with a minimum concentration of 5 ppm (Fig.1). During the H2S test, a two-step response of the sensor was recorded, which provided information for understanding the effects of chemisorbed and photo-induced oxygen species on the gas-sensing properties of the illuminated sensor. A possible light-induced gas-sensing mechanism of the SnO thin film was proposed and investigated in detail.

16:30 On the Role of the Device Geometry in the Gas Sensing Performance of Metal Oxide Nanowires **X.PI.23**

Authors : Roman Jiménez-Díaz (a,b); Albert Romano-Rodriguez (b); Olga Casals (b); Cristian Fábrega (b); J.Daniel Prades (b); Francisco Hernández-Ramírez (a,b)
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Resume : Metal oxides (MOXs) represent a significant fraction of research for developing solid state gas sensors. Here, the chemical-to-electrical transduction mechanisms between a reducing gas, carbon monoxide (CO), and an n-type metal oxide (SnO2) were theoretically evaluated and confronted to experimental data obtained with individual nanowires. Our analysis revealed that the sensing process has a complex nature with the concomitant contribution to the response of different experimental parameters such as the concentration of the target gas, the working temperature and the intrinsic properties of the nanowires, with a noteworthy role given to the device geometry, which fully determines the characteristics of the sensors. Those nanowires with thinner radii showed better performance not only in terms of the absolute response to a fixed gas concentration, but also bigger exponents in the power law dependence of the response as function of the gas concentration in air. On the basis of these results, it is clear that any meaningful assessment of the sensing properties of MOX nanowires needs to account for the device geometry influence on the final responses.

16:30 Influence of Annealing Temperature on Performance of on-chip hydrothermally growth ZnO nanorod gas sensor **X.PI.24**

Authors : Mingzhi Jiao*, Nguyen Van Duy**, Nguyen Duc Hoa**, Nguyen Van Hieu**, Klas Hjort*, Hugo Nguyen*
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Resume : Detection of harmful gases is not only important for monitoring of machine processes but also for monitoring of living environment. For both smell-free insidious gases, such as CO, CO2, and odorous gases, such as NO2, NH3, ethanol, it is important to know their concentration. Nanostructured materials (thin film, nanowires, nanorods, flakes, etc) have been enabling production of low-cost and low-power devices for gas sensing, yet research on synthesis and modification of these materials to render highly sensitive and selective sensor to specific gas is still being extensively carried out

worldwide. ZnO nanomaterials synthesized with hydrothermal method are very popular because of the very low requirement on equipment, but they have to be stabilized by annealing before use for gas sensing. Up to now, not much has been reported on influence of annealing temperature on sensing performance of the ZnO materials. This work focus on this ussue and NO2 is selected as target gas – a prominent air pollutant mostly from car combustion engines and thermal power stations. First, we fabricated gas sensors based on on-chip grown ZnO nanorods, then annealed them at 400, 500, and 600 °C for 4 hours. Gas sensing performance of the sensors was tested towards NO2. It was found that sensitivity of the gas sensors to NO2 decreased, but stability increased with the increase of annealing temperature. The reason may be found in the fact that annealing can lower the number of oxygen vacancy, an important defect for gas sensing, on the ZnO surface and increase its crystallinity at the same time. Annealing at higher temperature leads to lower defect density on the surface. The mechanism of the effect of annealing is being investigated by photoluminescence spectrometer and XRD.

16:30 Nanostructured TiO2-based gas sensors with enhanced sensitivity **X.PI.25**

Authors : W. Maziarz (a), A. Kusior (b), A. Trenczek-Zajac (b)
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Resume : The resistive-type gas sensors market is dominated by materials developed on the base of thin or thick layers composed of polycrystalline metal oxides. A new approach to the sensor technology is to use the nanomaterials. It is expected that they will provide better parameters than those of conventional materials. The nanostructures of different forms, i.e. wires, tubes, flowers, etc. were shown to display better gas selectivity and sensitivity. The high surface to volume ratio of such materials is responsible for this effect. Open nanostructures facilitate penetration of a gas which, in a consequence, reduces the response time. In this work, TiO2 nanostructures in a form of flowers were prepared by chemical oxidation and etching of Ti substrates. Compact, anodized TiO2 layers were used for comparison. Gas sensor responses were measured to acetone and nitrogen dioxide at different working temperatures and for varying gas concentrations. The results indicate the TiO2 anodized layers are more sensitive to acetone than to NO2. The response (S=Rair/Rgas) to acetone was S = 1.3@1.6ppm, S = 3@8ppm (360oC), while for NO2 it was lower (S=1.7@400 ppm). The response/recovery times for 8 ppm of acetone at 360oC were 12s/16s, respectively. For 400 ppm of NO at 360oC the corresponding times were 21 and 27s. The nanoflowers of TiO2-SnO2 exhibit extremely high sensitivity to acetone (S = 311@308oC but with longer response/recovery times (158 and 40 s respectively). Acknowledgement This work was financially supported by the Statutory project no. 11.11.230.016 of the Faculty of Computer Science, Electronics and Telecommunications, AGH-UST granted by the Polish Ministry of Science and Higher Education.

16:30 Studies and characterizations of oxidizing pollutants interactions on nanocarbons for filtering and sensing applications **X.PI.26**

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Resume : Nanocarbons constitute a wide range of materials with a high diversity of structures, morphologies and dissimilar surface chemistry. Physical or chemical treatments can modulate their characteristics making them suitable for many developments. Thus, innovations on electronic and optoelectronic components, supercapacitors or gas treatment units have been performed. If the interest of gas adsorption on nanocarbons is manifest for hydrogen storage or gas purification, their reactivity with air pollutants can be also exploited for the development of chemical filters and sensors. The modulation of the physical and chemical properties of nanocarbons is strategic to boost their filtering efficiency, to increase their durability and to improve their selectivity. The interactions of oxidizing pollutants on a large panel of nanocarbonaceous materials (tubes, fibers, cones, activated carbons) have been investigated. The physisorption of NO2 and the chemisorption of O3 on nanocarbons have been clearly established. Physical and chemical treatments on nanocarbons (grinding, graphitization and fluorination) were performed to modulate their gas adsorption properties. The specific surface area, density of dangling bonds and surface oxygenated groups (SOGs) were identified as the main factors of influence. Results about the implementation of nanocarbons as sensing or filtering materials for the development of sensor-systems devoted to NO2 monitoring in ppb-range will be specified.

16:30 A NEW CHEMICAL SENSING MATERIAL FOR ETHANOL DETECTION: GRAPHENE-LIKE **X.PI.27** ☆

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Resume : In this work, with the aim of realizing an ethanol device operating at RT, we have fabricated a chemi-resistive sensing layer based on a graphene related material (GRM): a so-called graphene-like (GL) layer. These materials are produced starting from a nanostructured carbon black through a two steps oxidation/reduction method under mild conditions and in aqueous environment. The GL layers undergo to self-assembling in thin film on surfaces after drying, driven by the instauration of hydrophobic interactions between the graphenic layers, as typically observed in reduced graphite oxide. Thanks to the presence of residual oxygen functional groups, mainly carboxylic groups, as confirmed by X-ray Photoemission Spectroscopy, atomically flat self-assembly over large areas is enabled at low pH. To assess the ability of the GL-based sensing layer to reveal low concentrations of ethanol at RT, the device was introduced into the gas testing chamber and exposed to 50 ppm of ethanol in dry N2, setting the voltage at 1 V. The device response is defined as the maximum variation of conductance recorded during the exposure of the sensing materials to controlled concentration of analytes, i.e Gmax-G0/G0 where G0 is the electric conductance in the initial unperturbed state. GL material is responsive to this analyte, exhibiting a response of 3% with a Signal-to-noise ratio (SNR) > 40dB. This result is even more astonishing when compared to the

detection limits of other devices operating at RT, reported in the literature. From the literature, pristine graphene emerges as totally insensitive to ethanol.

16:30 **Metal Functionalized ZnO Nanorods for Hazardous Gas Sensing at Room Temperature** **X.PI.28**

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Resume : In this study, one-dimensional nanostructured forms as nanorods of the pure and palladium doped with various dopant concentrations zinc oxide (ZnO) were fabricated on gold electrodes of the quartz crystal microbalance by electrochemical deposition techniques. Fabricated samples were tested to not only volatile organic compounds (VOCs) but also inorganic gas species as carbon monoxide (CO), sulphur dioxide (SO2) and hydrogen (H2) have fatal effects on human health. Sensor responses of the fabricated samples increased with increasing of the Pd dopant concentrations due to catalytic effects. Catalytic materials produce new impurities in the crystal structure of the metal oxide and enhance bond dissociations of the target molecules. Acknowledgement: This study was partly supported by TUBITAK (Grant No: 113F403 and 111M261) and by COST Action TD 1105 EuNetAir- European Network on New Sensing Technologies for Air Pollution Control and Environmental Sustainability- by a STSM year 2 (STSM-TD1105-16434, from 03-03-2014 to 28-03-2014): Functionalization of ZnO Nanorods With Metal and Metal Oxide For Gas Sensing Applications.

16:30 **Single crystalline oxide layers with defined doping to identify and improve the gas-sensing mechanism: The example of In2O3** **X.PI.29**

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Resume : Indium oxide is a well-known material for conductometric gas sensors, showing a decrease in conductance through exposure to to oxidizing gases such as ozone. These gases act as acceptors upon adsorption and can be desorbed by UV illumination. For traditionally-used polycrystalline layers the sensing mechanism has been described as a modulation of the depletion zone at the grain boundaries with major impact on the transport from grain-to-grain. In our contribution, single crystalline or textured In2O3

layers grown by molecular beam epitaxy (MBE) are used as simplified model systems to identify the fundamental gas sensing mechanism. Here, the total layer conductance is the sum of the bulk and surface conductance. The presence of a surface electron accumulation layer (SEAL) has been identified in MBE-grown In2O3. Its removal by an oxygen plasma treatment as well as the reduction of the bulk conductance by controlled Mg-doping allowed us to identify the SEAL as key of the gas sensing functionality as well as sensitivity improvements by Mg-doping. Hall measurements helped to estimate the SEAL electron concentration and mobility. Our results of using SEALs for gas sensing and bulk doping by deep acceptors to increase sensitivity can be generalized to other gas sensing materials. The use of single crystalline films allows selecting the most sensitive crystallographic surface orientation and may have further advantages over polycrystalline films, such as increased stability and sensing speed.

16:30 Metal Oxide based gas sensors operating at room temperature **X.PI.31**

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Resume : Sensing of hazardous gases is of great importance during the last decades. For this purpose many materials, mainly metal oxides, have been studied and tested in as far as their sensing characteristics are concerned. Zn and In oxides are well-known wide band gap semiconductors that are used in many applications due to their excellent optical, structural and electrical properties. Among them, their surface chemical sensitivity along with the variation of conductivity when reacting with oxidizing gases, such as ozone, makes them appropriate candidates as gas sensing materials [1]. In the present work, ZnO and In2O3 films were produced by dc magnetron sputtering method using a metallic targets, at room temperature. The materials were deposited on both glass substrates with NiCr contacts and Surface Acoustic Waves (SAW) filters [2] and were tested towards ozone via two different means; by recording conductivity changes and by monitoring the central frequency shift of the SAW filter, respectively. It was found that conductivity was decreased by several orders of magnitude in the presence of 10-100 ppb ozone concentrations at room temperature. Corresponding results regarding high frequency SAW filters (930MHz central frequency) revealed a frequency shift of a few MHz towards 1 ppm ozone pulses at 150°C. Elaboration of additional results and sensing performance on lower filter frequency SAWs will be presented. [1] M. Bender, E. Fortunato, P. Nunes, A. Marques, R. Martins, N. Katsarakis, V. Cimalla and G. Kiriakidis, “Highly Sensitive ZnO Ozone Detectors at Room Temperature”, Jap. J. Appl. Phys. 42 (2003). [2] G. Kiriakidis, K. Moschovis, I. Kortidis, V. Binas “Ultra-Low Gas Sensing utilizing Metal Oxide Thin Films” Vacuum 86 (2012) 495-506

16:30 Development of an impedancemetric Perchlorate microsensor with a picomolar detection limit based on nanostructured CoPc **X.PI.32**

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Resume : Perchlorate (ClO4-) contamination of public drinking water wells is now a serious problem in the world. The ClO4- anion is chemically stable and very soluble in water. High concentrations of perchlorate in potable water represent a potential health risk for human beings as it interferes with iodine uptake by the thyroid gland [1]. In this work, we will developed a miniaturized a ClO4- bio-chemical sensor based on a new nanostructured Co-phthalocyanine (CoPc) derivative functionalized Au microelectrode which morphological properties have been characterized by AFM. The response of the obtained sensor based CoPc/Au microelectrode has been investigated by Impedance spectroscopy measurements. The experimental impedance data of the sensor device were analysed by an equivalent electrical circuit using a modified Randles model for better understanding the phenomena present at the sensing membrane/electrolyte interface. Therefore, under optimized working conditions in terms of polarization and frequency, better performances have been achieved compared to those obtained for Au electrodes based devices functionalized with the same molecule: a lower detection limit (14.1 pM) and a larger linear range from 1.41 10-11 to 10-1 M were obtained. We have also studied the selectivity of our sensors by evaluating the response towards perchlorate with other interfering anions. Then, selectivity coefficients indicate a good discriminating ability towards ClO4– ion in comparison to other anions. These performances are better than those achieved in our previous works [2, 3]. References: [1] Alison M. Gardell el al, General and Comparative Endocrinology 219 (2015) 45–52. [2] M. Braik, et al, Organic Electronics 16 (2015) 77–86. [3] M. Braik, el al, J. Sens. Sens. Syst., 4 (2015) 17–23. Acknowledgements This work was partially supported by FP7-PEOPLE-2012-IRSES N° 318053: SMARTCANCERSENS and the NATO Science for Peace Project CBP.NUKR.SFP 984173.

16:30

Preparation and characterization of porous clay ceramic used to remove salt from the saline soils

X.PI.33

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Resume : This study was focused on the preparation and caracterizations of clay ceramics used as a tool to remove salt from the saline soils. The results obtained represent an interesting contribution to the knowledge of some aspects of ceramic porous in desalinisation methods. The used ceramics, mixes of kaolin and other suitable low cost materials such as quartz, sodium carbonate and calcium carbonate, were prepared by pressing and firing at 950–1150 °C. The studied samples as circular disks (≤50 mm diameter and ≤4 mm thickness) were subjected for characterization studies using ICP, XRD and SEM analysis before and after application, in order to evaluate and improve their efficiency in removing salt from soil. Pore size distribution, porosity, average pore size of the samples were carried out to study the ceramic performance, the importance of the pores

dimensions and structures on the solution movement and salt deposal. Moreover, a considerable decrease in the average pore size was observed with the desalination time (from 6µm to 1.2 µm). the samples porosity reduced also from 42% to 23%. Henceforth, these low cost ceramics with good properties are suggested for desalination processes.

16:30 CVD TRANSFER FREE GRAPHENE FOR SENSING APPLICATION **X.PI.34**

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Resume : Graphene-related materials have been widely explored for the fabrication of gas sensors because of their high conductivity and large specific surface areas. In this applicative scenario, we present graphene synthetized by transfer free Chemical Vapour Deposition (CVD). The multi-layer graphene was deposited using the CMOS compatible Mo as the catalyst, combined with a novel transfer-free fabrication method as described in detail elsewhere. The advantage of this method is that no transfer is needed and therefore during fabrication the graphene is not damaged or contaminated, as shown by the Raman data. Moreover, by pre-patterning the Mo catalyst graphene with different dimensions can be obtained. The sensing properties of material has been tested by exposing the device to different analytes. To this aim NO2 and NH3 have been selected because of the electron acceptor- and donor-like nature, respectively and the concentration ranges has been chosen by considering a realistic application of the device, i.e. 0,24-2,4 ppm for NO2 and 15-100 ppm for NH3. The measurements have been carried out in humid N2, setting the relative humidity (RH) at 70%, the flow at 500 sccm and the temperature at 22°C. The material proves to have a p-type nature, as an increase of the conductance response, in the range of 0.13%-1,57%, have been recorded upon exposure towards NO2, whereas a decrease of the signal, ranging between 0,26 and 0,75%, have been detected towards NH3.

16:30 AB-INITIO AND DFT STUDY OF FLUORINE AND CHLORINE SUBSTITUTED POLYACETYLENE ISOMERIZATION KINETICS **X.PI.35**

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Resume : To explain the isomerization reaction mechanism of substitued polyacetylenes, we used an HF (ab-intio) and DFT (B3LYP) 6-31G and 3-21G** methods. The various (rotations, conversions, rearrangemnts) and the different intermediates (transition state) were investigated. The results were as following: * The studied bonds in the fragments (C10H12, C10H6F6, C10H6Cl6) showed an important stability, justified by the low HOMO-LUMO energetic gap observed. However, the stability of many conformations showed that, the trans form was the more stable than the cis form. * The different reactions profiles, reveled that the size and the nature of the dopant (substituant) play a major role in the evolution of the activation energy. * The calculated activation energy values

indicated that the rates constants were in the order: kC10H12 >>kC10H6F6>> kC10H6Cl6. * Reaction intermediates during Cis-Trans transition showed that the geometrical parameters (angles and diedres angles) were amongst the most changed parameters, this was observed in the cases of substituted and unsubstitued PA.

16:30 The control of the structural properties of ZrO2 nanopowders via co-doping with Cu and Y **X.PI.36**

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Resume : The performance of ZrO2-based catalysts depends on their structure and stability. ZrO2 is known as a suitable support for Cu, which spatial localization is essential for the application of Cu-doped ZrO2 as lubricant, catalyst or fungicide. Among different ZrO2 phases, tetragonal one generally exhibits better catalytic properties. In this work the effect of Cu doping (1-8 mol%) on phase transformation in 3mol% Y-stabilized ZrO2 powders was studied. The powders synthesized by a co-precipitation technique from mixed Zr, Y and Cu nitrates and calcined at Tc=500-1000oC for 2 h. The samples were investigated by means of ATR-FTIR, diffused reflectance, XRD and TEM methods. It was found that the powders calcined at Tc=500-600oC shows mainly c-ZrO2 phase, while for Tc=700-800C the c-t transition occurs. With temperature increase the m-ZrO2 phase appeared. Similar effect was earlier observed for Y-ZrO2 powders and explained mainly by the increase of the ZrO2 grains [1]. Contrary to this, in (Y,Cu) codoped samples the t-m phase transformation is favored by the outward diffusion of Cu ions from ZrO2 grains and their precipitation at grain surface that is confirmed by diffused reflectance. This conclusion is supported also by the additional annealing followed by quenching resulted in the decrease of the content of Cu-related centers in the grains [2]. The obtained results are important for the catalysts application of (Cu,Y) codoped ZrO2 powders. 1. N. Korsunska, M. Baran, A. Zhuk, Yu. Polishchuk, T. Stara, V. Kladko, Yu. Bacherikov, Ye. Venger, T. Konstantinova, L. Khomenkova, Mater. Res. Express 1, 045011 (2014). 2. N. Korsunska, M. Baran, Yu. Polishchuk, O. Kolomys, T. Stara, M. Kharchenko, O. Gorban, V. Strelchuk, Ye. Venger, V. Kladko, L. Khomenkova, ECS J. Solid State Sci.Technol., 4(9), p. N103-N110 (2015).

16:30 AGD and DC Reactive Sputtering synthesis of WO3 thin films for gas sensors **X.PI.37**

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Resume : In the present work nanostructured WO3 films were deposited by DC Reactive Sputtering (DCMS) and Advanced Gas Deposition (AGD) methods on two types of electrical solid state sensors. Type A was a Si/SiO2 substrate with Au electrodes (100 nm thickness). Type B was a ceramic substrate with Pt electrodes (5 µm thickness). The thicknesses of films deposited on type A sensors were 125 nm (DCMS) and 320 nm (AGD). In case of type B sensors, the WO3 films were 1.4 µm and 25 µm thick, respectively. The

morphology and structure of the deposited films were characterized by profilometry, SEM and XRD, and their chemical composition analyzed by XPS. In each case the surface resistivity of the films were measured. Our results suggest that films prepared by AGD yield WO3 films with beneficial sensing properties, such as high porosity, controllable particle diameters, composition and structure.
Acknowledgement: This work was supported by A grant of the Romanian National Authority for Scientific Research, CNDI–UEFISCDI, project number 198/2012- SENSGAS UEFISCDI, the European Union's Horizon 2020 Research and Innovation program under grant agreement 645758 RISE-TROPSENSE 2015-2019, and the European Research Council under the European Community's Seventh Framework Program (FP7/2007–2013)/ERC, Grant Agreement No. 267234 ("GRINDOOR").

16:30

Novel Zwitterionic Polymer Modified Ag Nanocubes Based SERS Substrates as Sensitive Biosensors in Human Blood Serum

X.PI.38

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Resume : By FDTD simulation we observe that nanocubes have stronger electromagnetic enhancement between the gap of Ag nanocubes (AgNCs) and Ag film. As a result, robust surface-enhanced Raman scattering (SERS) substrates with hot spots generating from large-scale massive nanogaps between AgNCs and the Ag film via 1, 2-ethanedithiol monolayer as a linkage are fabricated. In real complex media such as human blood, SERS signals will be greatly interfered by biological substance adsorption which impedes analyte molecules and generates background noise. Therefore, we introduced the superhydrophilic zwitterionic polymer, PGMA-r-PSBMA and self-assembled it on the previously fabricated substrate. The sulfobetaine headgroup of zwitterionic polymer can bind water and resist biological adsorption. By coating this layer, the substrate can effectively resist adhesion of large biomolecules such as protein, bacteria, red blood cells and blood plate; meanwhile, it possesses proper pore size, allowing small detection molecules to diffuse into hot spot zones, leading higher S/N ratio of the sensor. In this work, we successfully utilize the modified SERS substrate to detect 0.5 ppm malachite green in human blood serum by 633 nm laser excitation, and the contact angle can reduce from 50°to 10°. The anti-biofouling ability is confirmed by confocal microscope and ELISA test. The results indicate that reliable zwitterionic polymer modified SERS substrate performs excellent detection in human blood serum.

16:30

Probing the role of Point Defects in sensing mechanism of chemoresistive Metal Oxide Gas Sensors

X.PI.39

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Resume : The thermodynamic stability of the system demands the formation of structural defects in real crystals. An 'ideal crystal' is the one, in which all the basis (atoms or ions) occupies the regular lattice points governed by the symmetry rules, to establish a long range periodic order. However, the real crystals differ from an ideal one, as it

contains a number of crystal defects. Here, we have investigated the crucial role of point defects (particularly the oxygen vacancies present in the metal oxide lattice), in the gas sensing mechanism of solid state metal oxide (MO) gas sensors. Often, while evaluating the basic mechanism of MO gas sensors, major attention is paid towards the physical size and dimensionality of the MO material rather than the defects, chemical stoichiometry and related attributes. Hence, it is necessary to consider this crucial aspect in order to develop the complete understanding of the chemoresistive MO gas sensors, which still seems to be far from reality. In this talk, the indirect spectroscopic ways such as Optical, Raman spectroscopy and X-ray photoelectron spectroscopy of characterizing the structural point defects are discussed. The defects which are further tuned and utilized in understanding their effect on the gas sensor mechanism. To summarize, the talk shall present a novel perspective to understand the mechanism of the metal oxides semiconductor gas sensor operation, through probing the defect structure. Albeit, there is a wealth of a literature published in the field of MO gas sensors in last few decades, the approach of the researchers has been empirical, which could be a limiting factor for further advancement in the field. Hence, one needs to be more keen to study the structural aspects to obtain a colossal improvement. The only possible approach could be, to gain more insight into the mechanism and standardizing the criteria for choice of materials thereof. Here, the mechanism involved in the MO chemoresistive gas sensors is discussed in detail and the prime focus on effect of structural defects, which influence this mechanism significantly.

16:30 HYBRID NANOSTRUCTURES FOR THE DETECTION OF THE VOLATILE ORGANIC COMPOUNDS **X.PI.40**

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Resume : Human expired breath contains different types of volatile organic compounds (VOCs) resulted from the metabolic process. Despite their low concentrations (parts per million or parts per trillion by volume), these species can provide an indication of certain illnesses, allowing a distinction between healthy and diseased states. Although gas chromatography (GC) has been widely used for the analysis of VOCs, more recently, new gas sensor devices based on conducting polymers have been developed. Among these polymers, polyaniline (PANI) was found to be sensitive to a wide range of VOCs contained in expired breath. The purpose of our work is to develop new hybrid nanostructured thin films based on PANI and Au nanoparticles using hydrothermal-electrochemical method. HAuCl4 and commercial PANI in the form of emeraldine were used as raw materials for the deposition of nanostructured thin films on two types of substrates: Si/SiO2/Au and cover glass/Au, respectively. The resulted hybrid thin films were characterized by surface analysis methods such as scanning electron microscopy (SEM), atomic force microscopy (AFM) and Fourier transform Infrared spectroscopy (FT-IR). Potential application of PANI/Au thin films as VOCs biosensor will be evaluated. Acknowledgments: 1. By Horizon H2020 - Marie Sklodowaska - Curie (MSCA) Research and Innovation Staff Exchange (RISE) Tropsense ?Development of a non-invassive breath test for early diagnosis of tropical diseases?

16:30 Benzene and its derivatives detection with ethylene vinyl acetate – nanostructured carbon composite

X.PI.42

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Resume : In our previous research sensoreffect on various petrol samples (vapours) has been detected. In order to explain the sensoreffect gas chromatography of samples was done. Results showed that more than 60% of petrol (with octane number 95) content was benzene derivatives, like toluene, 1,3-dimethylbenzene and ethylbenzene. Many countries including Latvia has determined that pure benzene content in fuel has to be below 1%. Benzene is found in the vehicle exhaust as well, as other hydrocarbons, which were present in the original fuel. OSHA (Occupational Safety and Health Administration) has determined the legal airborne permissible exposure limit (PEL) for benzene at 1ppm (averaged for 8-hour work day) and 5ppm for 15-minute exposure [1]. As a sensor material was used nanocomposite made of ethylene vinyl acetate copolymer filled with conductive carbon nanoparticles (EVA-CB). Ethylene vinyl acetate copolymer (EVA; Sigma Aldrich) with vinyl acetate content 40% was used as polymer matrix for the nanocomposite. Carbon nanoparticles (CB; PRINTEX XE-2) with average particle size 30 nm was used as conductive filler. As mentioned before more than 60% of petrol is benzene derivatives and benzene content is regulated in many countries, therefore EVA-CB response on benzene and few of its derivatives is evaluated. There is determined minimal vapour concentration, which can be distinguished in air with EVA-CB, repeatability of sensoreffect, response time and recovery time at wide range of vapour concentrations were tested as well. References: [1] Occupational Safety and Health Standards, Part Number: 1910, subpart: Z, Toxic and Hazardous Substances, Standard Number: 1910.1028, Benzene

16:30 Conduction mechanism in gas sensors based on ZnO nanowire networks

X.PI.43

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Resume : Conductometric metal-oxide based gas sensors are widely used today due to their high sensitivity. A further improvement has been proposed by using metal-oxide nanowires due to the large surface over volume ratio. In this direction, ZnO nanowires grown in liquid phase have shown advantages due to their superior stability owing to high crystallinity, simple and low-cost preparation methods, and wide variety of morphologies. Recently, gas sensors based on nanowire networks drop-casted or spin-coated on electrodes have been demonstrated, but their sensing mechanism, related to the transport through the nanowire network, is still weakly investigated. Here we investigate the electrical transport in sensors based on ZnO nanowire networks, realized by depositing a solution of ZnO nanowires grown in liquid phase on predefined electrodes with different geometries. By varying the geometry of the electrodes, we are able to distinguish the effect of transport barriers occurring at the electrodes to barriers occurring at the nanowire-to-nanowire junctions. The conduction through the ZnO nanowire networks is compared to models of conduction though polycrystalline thin film metal oxide sensors in order to model their sensitivity, and we investigate the influence of sintering the nanowires through annealing in different

atmospheres. These analyses are important in order to determine the sensing mechanism of conductometric sensors based on nanowire networks.

16:30 Phtylocyanine thin film/TiO2 nanotubes hybrid for VOC sensing at room temperature **X.PI.44**

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Resume : Abstract This work presents gas sensing properties of Phthalocyanine thin films/TiO2 nanotubes heterostructure. Highly-ordered TiO2 nanotubes were grown by the anodization of titanium foil [1]. Then the nanotubes were annealed at 300 ºC for 5 h in the ambient dry air to obtain crystallized TiO2. After that (C6S)8PcM (M=2H, Ni, Cu, Zn) phthalocyanines solved in chloroform were coated by spray process on annealed TiO2 nanotubes. Film thickness of phthalocyanines were almost 25 nm. The morphologies and structure of the samples were characterized by X-ray diffraction (XRD), scanning electron microscope (SEM). TiO2 nanotubes have an anatase crystal structure and 90 nm in diameter. Phtyalocyanine films were homogenously covered on all oxide surface. VOCs sensing properties of Phthalocyanine thin films/TiO2 nanotubes heterostructure were investigated at room temperature under nitrogen (N2) ambient used due to better understand the effect of heterostructure on gas sensing. The conductivity of phthalocyanines increases under the flow of oxygen, which is getting harder how the sensing mechanism of heterostructure is. The results showed that the sensor response of heterostructures is better than that of phthalocyanine thin films [2]. Acknowledgement: This study was supported by The Scientific and Technological Research Council of Turkey (TUBITAK) with project number of 113F403. References 1. Erdem Şennik et al., “Synthesis of highly-ordered TiO2 nanotubes for a hydrogen sensor”, International Journal of Hydrogen Energy, 35 (2010) 4420–4427. 2. F. Siviero et al., “Hybrid n-TiO2-CuPc gas sensors sensitive to reducing species, synthesized by cluster and supersonic beam deposition”, Sensors and Actuators B: Chemical, 126 (1) (2007) 214-20.

16:30 SnO2 NWs network site-selectively synthesised as ammonia sensor in dry and humid air **X.PI.45**

Authors : Jordi Samà 1, Sven Barth 2, Guillem Domènech-Gil 1, Joan Daniel Prades 1, Nuria Lopez 3, Olga Casals 1, Francisco Hernández-Ramírez 1 4, Isabel Gràcia 5, Carles Cané 5, Albert Romano-Rodríguez 1
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Resume : Nanostructures as nanowires (NW) or nanotubes (NT) are highly interesting morphologies for gas sensors due to the high surface to volume ratio [1], which leads to enhance the transduction of the interaction between their surface and the surrounding gas molecules into a change in their electrical resistance. An important drawback of fabricating electronic devices based on nanowires as building blocks using bottom-up approaches is the integration, which is difficult, time consuming and expensive. Site-selective growth of SnO2 has been performed on top of CMOS compatible micromembranes that contain a microheater which provides the thermal energy necessary for the growth. Synthesis of NWs is carried out by a localized Chemical Vapor Deposition process using Au as a catalyst, in a fast, and low power consumption process. The network of NWs is fabricated on micromebranes without employing a mask and no post-processing is needed to use the network as a gas sensor. The SnO2 NWs-based devices have been characterized towards several tens of ppm of NH3 in dry and humid conditions. The ammonia response is diminished and slowed down in presence of water vapour. The sensing kinetics at different temperatures have been analysed, allowing to identify the concurrent mechanisms. A response time of less than a minute and good repeatability of ammonia response are obtained from the characterization of the sensor. References [1] Satyanarayana V.N.T. et al. (2007) “One dimensional nanostructured materials”, Progress in Materials Science 52, 699-913.

16:30

Room temperature humidity sensing of NiO films, electrospun NiO nanofibers and NiO nanofibers/NiO films systems

X.PI.46

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Affiliations : a) Energy Technologies Department, ENEA Casaccia,Via Anguillarese 301, 00123 Rome, Italy; b) Italian Interuniversity Consortium on Materials Science and Technology (INSTM), Research Unit Roma Tor Vergata, Via del Politecnico 1 - 00133 Rome, Italy; c) Italian National Research Council, Institute of Atmosferic Pollution Research, Via Salaria 300, Monterotondo, 00015 Rome, Italy; d) Department of Enterprise Engineering, University of Rome Tor Vergata, Via del Politecnico 1 - 00133 Rome, Italy

Resume : The electrical response towards relative humidity variations of electrospun nickel oxide nanofibers, oxidized sputtered nickel films and a multilayer systems made of NiO nanofibers on NiO films was measured. Polyvinylpyrrolidone/Nickel (II) acetate precursor fibers were directly deposited by electrospinning on radio frequency (r.f.) sputtered thin Ni films grown on quartz substrate and Au/Cr interdigitated electrodes on alumina substrates. The samples were calcined in air at 500°C for 90 min to obtain NiO nanofibers and NiO nanofibers/NiO films systems. NiO samples were obtained by r.f. sputtering of a Ni target in Ar+O2 atmosphere or by post deposition annealing (500 °C, 90 min) of r.f. sputtered Ni films. Morphological and structural properties of the different samples were investigated by SEM and XRD analysis. Preliminary electrical and chemiresistive measurements performed at relative humidity values in the range 0-80% showed a different behavior of NiO nanofibers with respect to NiO nanofibers/NiO films. An high and rapid response to humidity values greater than 40% was observed in the first case.

16:30 Gas sensing characteristics of thin film SnO2-ZnO composite metal-oxide semiconductor sensors **X.PI.47**

Authors : P. Chesler1, C. Hornoiu1, M. Gartner1, S. Mihaiu1, M. Zaharescu1, C. Moldovan2, B. Firtat2, I. Stan3
Affiliations : 1 “Ilie Murgulescu” Institute of Physical Chemistry of the Romanian Academy, 060021 Bucharest-Romania; 2 National Institute for Research and Development in Micro-technologies, 077190 Bucharest - Romania; 3 Romelgen SRL, Bucharest – Romania;

Resume : A series of bi-component SnO2-ZnO metal oxide thin films were deposited on a gold inter-digital electrode micro-structure supported by porous alumina. The sensors with different SnO2:ZnO ratios were prepared by sol-gel dip-coating, a low cost technology. Different gases were tested (CO, CH4, C3H8) in various concentrations on a wide detection range (200-2500 ppm). The gas sensing measurements (sensor sensitivity, response time, selectivity and recovery) were performed in environmental conditions (carrier gas is air) at different working temperatures (130-300 degrees C). The gas-sensing behavior of the films was correlated with the structural, chemical and morphological properties of the multi-layered structures. It was found that the sensor sensitivity is less dependent on the film thickness but is significantly influenced by the SnO2/ZnO ratio at the working temperature. For the composite sensor containing 2% SnO2-98% ZnO a sensitivity value of 22 for CO at a low working temperature of 170 degrees C is reported. Humidity sensing tests at room temperature were also carried out, with excellent results for the sensor containing 98%SnO2 – 2% ZnO (S=53). The response time was between 20-100 seconds and the recovery time was about 180 seconds for all the sensors.

16:30 Fabrication and gas sensing characteristics of CNT/metal hybrid gas sensors **X.PI.48**

Authors : Yong Jung Kwon, Sung Yong Kang, Myung Sik Choi, Jae Hoon Bang, Hyoun Woo Kim
Affiliations : Department of Materials Science and Engineering, Hanyang University, 222 Wangsimni-ro, Seongdong-Gu, Seoul, 133-791, Korea

Resume : Carbon nanotubes (CNTs) have been tested in devices and systems. There are remarkable characteristics of CNTs like large surface area, small size, hollow geometry, and highly sensitive electrical properties. We have prepared metal-CNTs hybrid nanostructures by sputtering technique with metal targets, subsequently investigating the effects of thermal annealing. The surface of hybrid metal-CNTs became uneven by thermal annealing, and being attributed to the agglomeration of the shell layers into the metal nanoparticles. The hybrid metal-CNTs were investigated by scanning electron microscopy, transmission electron microscope and x-ray photoelectron spectroscopy. Carbon nanotube (CNTs) based gas sensors have many possibilities because of their potential for the selectivity and rapid detection of various gases with low power consumption. The successful application of CNTs in gas sensors will contribute to the development of nanostructure gas sensing devices. This study is comprised of our previous literature (Sens. Actuators B 227 (2016) 157).

16:30 SILVER DECORATION OF GRAPHENE FOR EFFECTIVE TUNING OF THE SENSING SPECIFICITY **X.PI.49**

Authors : Maria Lucia Miglietta1, Brigida Alfano1,2, Tiziana Polichetti1, Ettore Massera1, Chiara Schiattarella2 and

Girolamo Di Francia1
Affiliations : 1 ENEA C.R. Portici P.le E. Fermi 1, I-80055 Portici (Naples), Italy 2 Department of Physical Sciences University of Naples Federico II Via Cinthia, I-80126, Naples, Italy

Resume : The unusual combination of singular properties in the same material made graphene an ideal candidate for sensing applications. As pristine material, graphene shows a high specificity towards electron acceptor molecules but its chemical reactivity can be further expanded towards different analytes by proper functionalization. In particular, it is known that decoration by silver nanoparticles (Ag NPs) improves the sensing behavior of carbon nanostructures towards ammonia. Herein, graphene/Ag nanoparticles (GR/AgNPs) hybrids were prepared by a one-step microwave-assisted reduction of AgNO3 in a water/isopropanol solution of graphene. By varying the silver precursor concentration, hybrids with different surface coverage were obtained and characterized by SEM, AFM and Raman spectroscopy to assess the effective decoration and the graphene surface coverage by Ag NPs. In addition, the sensing performances towards NO2 and NH3 were investigated in a Gas Sensor Characterization System. The results presented herein, showed that, at the highest surface coverage an almost complete reversal of the sensitivity from NO2 to NH3 with respect to bare GR occurs. A lower areal density of Ag NPs allows instead the material to keep the sensitivity to both the analytes. Therefore, by simply acting on the Ag NPs concentration, it was possible to retain the specificity to both the analytes or to completely switch it, attaining a material highly sensitive to NH3.

16:30 Three-nanosensor array microsystem to monitor infections **X.PI.50**

Authors : P. I. Gouma, J. Huang, Y. Lin and M. Stanacevic
Affiliations : Center for Nanomaterials and Sensor Development, SUNY Stony Brook, NY, USA

Resume : A three-sensor array consisting of a NO (nitric oxide), and ammonia, and an isoprene sensor has been developed into a breathalyzer system for detecting viral infections. This work focuses on the NO sensor in the array, the processing of the sensing element by a scalable nano-manufacturing process, and the performance of the sensor in the breathalyzer device. Detection of NO down to 200 ppb within a few seconds has been demonstrated. This is consistent with the detection limit required for the targeted application. The sensor’s response and long-term stability has been evaluated by testing (a number of sensors from the same batch of processed material) over the course of 6 months.

16:30 Superficial modification effects by catalysts on the gas sensor response of SnO structures **X.PI.51**

Authors : P.H. Suman(1,2), M.S. Barbosa(1), J.A. Varela(1), H.L. Tuller(2) and M.O. Orlandi(1)
Affiliations : (1) Department of Physical-Chemistry, São Paulo State University, Araraquara, SP14800-060, Brazil. (2) Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139, USA.

Resume : Growing concerns about the impact of gas emissions on health, safety and the environment have focused the researches for the development of new faster and more sensitive gas sensor devices to be able to detect low levels (ppm and even ppb) of flammable and toxic gases coupled with high long-term stability and selectivity for

potential interferents. Metal oxide semiconductor (MOS) based sensors have received a great deal of attention given its good performance combined with low cost materials and simple device design. However, improvements on the gas sensor properties of MOS can be achieved by addition noble metal nanoparticles (Au, Ag, Pt, Pd) which act as catalysts influencing the gas adsorption processes on the surface of the host material. In this work, we studied the effects of surface functionalization of tin monoxide materials by using noble metal nanoparticles (Pd and Ag). SnO micro-disks were synthesized by carbothermal reduction method in an inert synthesis atmosphere whereas Pd and Ag nanoparticles (NPs) were synthesized by a Polyol method through chemical reduction reactions. The surface modification of the structures was achieved by adding 1%wt metallic nanoparticles to the surface of the oxide structures followed by a thermal treatment. Morphological and structural characterization by high-resolution scanning and transmission electron microscopy (FE-SEM and TEM) indicated that well-dispersed Ag and Pd nanoparticles (with average diameters of 13 and 11 nm, respectively) were successfully deposited over the surface of the SnO structures. Gas sensing tests on both pure and modified structures were carried out by monitoring changes in the electrical resistance during cyclic exposure to different concentrations of analyte gases (NO_2, H_2 and CO) in different operating temperatures (100-350°C) using synthetic dry air as baseline gas. Differences in the electrical features of the multiple samples were observed and their gas sensor properties (sensitivity and selectivity) were altered by the surface modification. This effect can be attributed to the role of metal nanoparticles which acted as catalysts in the interaction of the oxide with reducing gases (H_2 and CO) and as deactivators in the interaction with NO_2, suggesting that chemical or electrical sensitization took place. Impedance Spectroscopy was also used to further investigate those processes, so that a model for the effects of metal catalysts could be proposed. Thus, the results suggest that, in specific conditions, pristine and metal-decorated SnO micro-disks show great promise to be used as an alternative gas sensor material.

16:30 Single Ga_2O_3 NW-based gas sensors **X.PI.52**

Authors : Guillem Domènech-Gil1, Jordi Samà1, Irimina Peiró-Riera1, Paolo Pelegrino1, Sven Barth2, I. Gracia3, C. Cane3, Albert Romano-Rodriguez1
Affiliations : 1. Universitat de Barcelona (UB), MIND-Departament dElectrònica and Institute of Nanoscience and Nanotechnology (IN2UB), E-08028 Barcelona, Spain 2. Vienna University of Technology (TUW), Institut für Materialchemie, A-1040 Vienna, Austria 3. Consejo Superior de Investigaciones Científicas (CSIC), Centro Nacional de Microelectrónica, Institut de Microelectrònica de Barcelona (IMB-CNM-CSIC) 08193 Bellaterra, Spain

Resume : Gallium oxide nanowires have been fabricated via a VLS process in a chemical vapor deposition (CVD) furnace by using carbothermal reduction of gallium oxide nanopowder, which allows the reduction of the required high decomposition temperature of the oxide. In this experiment the carrier gas has been argon gas. As a function of the distance from source material to the substrate, in a downstream configuration, different nanostructures and shapes have been obtained. Nanowires, one of them, have been obtained and tend to grow either in a 2D web distribution or vertically, and nanoplateletes. In this work we have structurally and optically characterised the synthesised nanowires using X-ray diffraction, scanning and transmission electron microscopy, as well as photoluminescence and Raman spectroscopy, confirming their monocrystalline and relatively defect-free nature. To study the gas sensing properties, the nanowires

were removed from the substrates where they grew using sonication and were further deposited on top of suspended microhotplates with buried heater and prepatterned electrodes and individual nanowires were contacted by combined Focused Electron- and Focused Ion-Beam assisted deposition techniques. The gas sensing behaviour of the obtained towards different gases relevant in air quality monitoring and as a function of the operation temperature will be reported.

START AT	SUBJECT	View All	NUM.	ADD

Functional Materials for Environmental Sensing : Hossam Haick

09:00 **CVD grown n-type metal oxide nanowires decorated with p-type core-shell nanoparticles for the detection of traces of environment** **X.II.1**

Authors : Sergio Roso, Toni Vilic, Eduard Llobet
Affiliations : MINOS-EMaS, Universitat Rovira i Virgili, Avda. Països Catalans, 26, 43007 Tarragona, Spain

Resume : Recently, we have shown how CVD is an effective and easily scalable method for growing hybrid metal oxide nanomaterials. In particular, it allows for functionalizing metal oxide nanowires with metallic nanoparticles (NPs) as an effective way for tailoring their gas sensing properties [1,2]. Here, we report on how tungsten oxide nanowires or indium oxide nano-octahedra can be made highly selective to some gaseous species by decorating these n-type nanomaterials with p-type core-shell nanoparticles of late transition metals/ metal oxides. Full details will be given on the growth and characterization of these hybrid nanomaterials together with their integration in transducers for resistive gas sensors. Their response, sensitivity and selectivity to some pollutants (e.g., hydrogen sulfide, nitrogen dioxide, etc.) or energy-relevant gases such as hydrogen will be shown, with special emphasis on these properties when nanomaterials are operated at low temperatures, including room temperature. The gas sensing mechanisms will be discussed, including the roles of both electronic and chemical sensitization played by core-shell nanoparticles, and the observed humidity de-sensitization will be justified in light of the experimental findings. [1] S. Vallejos, P. Umek, T. Stoycheva, F. Annanouch, E. Llobet, X. Correig, P. de Marco, C. Bittencourt, C. Blackman, Advanced Functional Materials, 23 (2013) 1313–1322. [2] F.E. Annanouch, Z. Haddi, S. Vallejos, P. Umek, P. Guttmann, C. Bittencourt, E. Llobet, ACS Appl. Mater. Interfaces, 7 (2015) 6842–6851.

09:30 **Detection of heavy metals using epitaxial graphene on SiC** **X.II.2**

Authors : Ivan Shtepliuk, Volodymyr Khranovskyy, Jens Eriksson, Anita L. Spetz, Rositsa Yakimova
Affiliations : Linkoping University, Department of Physics, Chemistry, and Biology (IFM), 583 81, Linkoping, Sweden

Resume : Due to ever-increasing industrial activities, agriculture and urban waste waters, toxic heavy metals (HMs) such as mercury, cadmium and lead are released in environment. These substances can cause detrimental effects on the ecosystem and human health. In this regard, it is very important to develop portable and fast sensors for monitoring HMs. Graphene having extremely low electronic noises, high

signal-to-noise ratio and large surface area is considered as an ideal candidate for chemical sensors. Recent success in epitaxial growth of high-quality and large-scale graphene layers by thermal decomposition of silicon carbide (SiC) has attracted special attention because of a possibility to use an unintentionally formed Gr/SiC junction as a sensing platform. Here we propose a new sensing mechanism driven by a fast change of intrinsic graphene properties and, as a consequence, barrier height of Gr/SiC junction due to charge transfer between graphene with incoming adsorbates such as Cd2+, Hg2+ and Pb2+. Such an interaction leads to modification of electrical properties of Gr/SiC junctions. Thus, we measured and analyzed the shift of the capacitance-voltage (C-V) curves and current-voltage (I-V) characteristics of the Gr/SiC devices, in which detection of heavy metals is enabled. The detailed carrier transport mechanisms occurring at two-dimensional (2D) graphene/ three -dimensional (3D) SiC interface under the influence of the HMs is comprehensively studied and discussed.

09:45 COST Action TD1105: New Sensing Technologies for Air-Pollution Control and Environmental Sustainability **X.II.3**

Authors : Michele Penza - on behalf of EuNetAir Consortium
Affiliations : ENEA, Italian National Agency for New Technologies, Energy and Sustainable Economic Development Lab Functional Materials and Technologies for Sustainable Applications - PO Box 51 Br4; I-72100 Brindisi, ITALY

Resume : This is a overview of the COST Action TD1105 EuNetAir - European Network on New Sensing Technologies for Air-Pollution Control and Environmental Sustainability - funded in the COST framework. The objective of the Concerted Action (2012-16) (www.cost.eunetair.it) is to develop new sensing technologies for Air Quality Control at multidisciplinary scale by coordinated research on nanomaterials, sensor-systems, air-quality modelling and standardised methods to support environmental sustainability with special focus on SMEs. This international Networking, coordinated by ENEA (Italy), includes over 120 institutions and over 200 international experts from 31 COST Countries (Austria, Belgium, Bulgaria, Croatia, Czech Republic, Denmark, Estonia, Finland, France, Germany, Greece, Hungary, Iceland, Ireland, Israel, Italy, Latvia, Luxembourg, The Former Yugoslav Republic of Macedonia, Netherlands, Norway, Poland, Portugal, Romania, Serbia, Slovenia, Spain, Sweden, Switzerland, Turkey, United Kingdom) and 7 Non-COST Countries (Australia, Canada, China, Morocco, Russia, Ukraine, USA) to create a S&T critical mass in the environmental issues. This COST Action [1-4] focuses on a new detection paradigm based on sensing technologies at low cost for Air Quality Control and set up an interdisciplinary top-level network to define innovative approaches in sensor nanomaterials, gas sensors, devices, wireless sensor-systems, distributed computing, methods, models, standards and protocols for environmental sustainability within the European Research Area. [1] M. Penza et al., Procedia Engineering, 2015, 120, 476-479 [2] M. Penza et al., Procedia Engineering, 2014, 87, 1370-1377 [3] M. Penza et al., Proceedings IEEE SENSORS 2014, 1-7. DOI: 10.1109/ICSENS.2014.6984918 [4] M. Penza et al., AMA Science, Open Access. DOI: 10.5162/4EuNetAir2015/01

10:00 *Coffee break*

Metal Oxide Nanostructures for Gas Sensing II : Jens Eriksson

10:30 Nanowires Metal Oxides as Environmental Chemical Sensors **X.III.1**

Authors : E.Comini, A. Bertuna N. Kaur , D. Zappa, V. Sberveglieri, G. Sberveglieri
Affiliations : SENSOR, Dipartimento di Ingegneria dell'Informazione, Università degli studi di Brescia e CNR-INO, via Branze,38, Brescia, Italy

Resume : A chemical sensor consists of a physical transducer i.e., a transducer of physical quantities into convenient output signals, and a chemically selective layer so that measurable output signals can be produced in response to chemical stimuli. It is often the physical transducer that imposes both fundamental and practical limitations on the performances achievable with chemical sensors. As a result, implementation of a transduction principle or innovative transducer design is always a significant milestone in the area of chemical sensors. New effects discovered at the nanoscale allow new perspectives on chemical sensor transduction. Miniaturization of a sensor down to a single nanostructure unit is not only a useful test for the fundamental limit of detection, but, most importantly, represents a promising approach towards real-time detection of single binding events, which is a key issue for future research in chemistry, biology and medicine. For commercial success, major advances in sensor technology are required in terms of simple structure, lower cost, selectivity, durability, and reliability. The most suitable sensors of these types are based on semiconductors that do not undergo irreversible chemical reactions forming stable oxides upon exposure to air at high temperature. Metal oxide gas sensors offer better stability and sensitivity as compared to other organic materials like polymers. The fundamental sensing mechanism is based on atmosphere changes closed to the active material, which leads to variations in the electrical or optical properties. Application of metal oxides as chemical sensors exploiting novel architectures for environmental monitoring will be reviewed as well as other application like food safety by a novel Electronic Nose

11:00 NH3 sensing with self-assembled ZnO-nanowire μHP sensors in isothermal and temperature-pulsed mode **X.III.2**

Authors : Feng Shao (a,b); Jian D Fan (a,c); Francisco Hernandez-Ramírez (a,d); Cristian Fábrega (d); Teresa Andreu (a); Andreu Cabot (a); J. Daniel Prades (d); Nuria López (e); Florin Udrea (f,g); Andrea D Luca (f); Syed Z Ali (g); Joan R Morante (a,d)
Affiliations : a. Catalonia Institute for Energy Research (IREC), Sant Adrià del Besòs E-08930, Spain b. School of Electronic Science and Engineering, Nanjing University, Nanjing 210023, China c. Clarendon Laboratory, University of Oxford, Parks Road, Oxford OX1 3PU, United Kingdom d. Department of Electronic, University of Barcelona, Barcelona E-08028, Spain e. Institute of Chemical Research of Catalonia (ICIQ), Tarragona 43007, Spain f. Department of Engineering, University of Cambridge, Cambridge, United Kingdom g. Cambridge CMOS Sensors Ltd, Cambridge, United Kingdom

Resume : Dielectrophoretic (DEP) alignment is found to be a simple and efficient method to deposit metal oxide nanowires onto micro hot plate substrates (μHPs). In this work, ZnO nanowires deposition onto μHPs was further developed by applying the DEP alignment at the post CMOS wafer stage. The response to ammonia (NH3) was evaluated in isothermal and temperature-pulsed operation mode; the relative higher response observed in the latter case demonstrates that the use of this methodology is a good strategy to improve the performance of metal oxide sensors based on nanomaterials. Here, we evaluate the response to NH3 and qualitatively describe the sensing mechanism in temperature-pulsed mode,

highlighting the main differences compared to the standard isothermal methodology. Sensors and Actuators, B: Chemical, Vol 226, 1 April 2016, Pages 110-117

11:15 Nanowire-based microsensors and the influence of the bottom-electrode configuration in the performance and reliability of gas de **X.III.3**

Authors : S. Vallejos, I. Gracia, O. Chmela, E. Figueras, J. Hubalek, C. Cané
Affiliations : SIX Research Centre, Brno University of Technology, 601 90 Brno, Czech Republic Instituto de Microelectrónica de Barcelona (IMB-CNM, CSIC), 08193 Cerdanyola, Barcelona, Spain

Resume : Nanowire-based microsensors and the influence of the bottom-electrode configuration in the performance and reliability of gas detection. ___ Chemoresistive micromachined gas sensors with bottom electrode configuration and based on a film of Pt-functionalized tungsten oxide nanowires were fabricated. The performance and reliability of three types of devices with different electrode gap (5, 10 and 15 µm) were analized in dry and humid ambients and towards various target analytes (H2, NO2, EtOH, and CO). The films composed of functionalized nanowires were directly integrated with the micromachined platfforms using the single-step method based on aerosol assisted chemical vapour deposition described previously [1]. Tests of the sensors were perfomed along 140 days during which the same sensors were alternatively subjected to the target analytes at different concentrations and operating temperatures, carrying out several replicates (overall, the array of sensors accumulated a total of 900 h of operation during the testing period). Results demonstrated improved sensitivity, cross-sensitivity, stability and dinamic of the sensor response for the sensors with narrower spacing (5 µm), indicating, for instance to hydrogen, up to 7-fold higher responses and 32-fold faster responses with relative better stability compared to the sensors with wider spacing (10 and 15 µm). These results were attributed to the increment of the density of nanowire junctions across the narrower electrodes; the junctions enhance not only the conduction channel of the networked wires, but also increase the potential barriers, which play an important role in the gas sensing mechanism of the overall film. [1] Adv. Funct. Mater. 2013, 23, 1313

11:30 Response of indium oxide nano-octahedra activated by switching UV light **X.III.4**

Authors : Oriol González, Sergio Roso, Eduard Llobet, Xavier Vilanova
Affiliations : MINOS-EMaS, Universitat Rovira i Virgili, Tarragona, Spain

Resume : In this paper, we focus in the transient gas response analysis of nano octahedral indium oxide while activated by switching UV light. The response kinetics towards oxidizing species (e.g., NO2) are highly increased. In2O3 octahedra has been synthesized by a vapor phase transport method in a chemical vapor deposition (CVD) furnace. The precursor used was a powder of metallic In (99.99%) and Ar gas was used as a carrier gas. Both, the precursor and the Si/SiO2 substrates were placed onto a quartz boat into the horizontal CVD. Then, the temperature was raised to 900ºC and kept constant during 2 hours. All the process was carried out under atmospheric pressure. The deposited material was removed by scratching the material from the substrate. Then a printable ink was prepared by mixing it with appropriate solvents and the materials was deposited by screen printing technique on top of a ceramic hotplate substrate with Pt electrodes on one side and a heater on the other side. Gas mixing and delivery were

performed by employing a computer controlled mass flow system. The sensors were placed in a home-made Teflon chamber, where the UV leds (325 nm) were also placed. Although under continuous UV light the response to NO2 is worse than when the sensor is heated, switching on/off the UV light allows for obtaining good responses in a faster way and with reduced power consumption.. The capacity of UV light to clean and desorb the species adsorbed on the surface of metal oxides has been reported. Here, we have studied the transients of oxidation (when UV is Off) and transients of reduction or cleaning (UV on) of the indium oxide surface in the presence of nitrogen dioxide diluted in air. Both processes combined create a ripple in the output signal (resistance) and this ripple has a different amplitude as a function of NO2 concentrations. Focusing in the periods when the UV light is switched off (i.e., when NO2 oxidizes the active layer), and analyzing the change rate of the material resistance, the gas concentration can be also determined, but in a faster way than when the sensor is operated at a fixed working temperature. In this study we will show the results when using different duty cycles for UV modulation (80%, 50% and 20%) where we can analyze and compare the UV cleaning effect obtaining a fast response for detecting NO2 at room temperature using an In2O3 based sensor.

11:45 Near Infrared Plasmonic Gas Sensing with Doped Metal Oxide Nanocrystals **X.III.5**

Authors : M. Sturaro1, E. Della Gaspera2, M. Guglielmi1, A. Martucci1
Affiliations : 1 Dipartimento di Ingegneria Industriale, Universita' di Padova, Italy. 2 CSIRO Manufacturing Flagship, Clayton, Australia

Resume : Highly doped wide band gap metal oxides nanocrystals have recently been proposed as building blocks for applications as transparent electrodes, electrochromics, plasmonics and optoelectronics in general. Here we show that the dopant-induced plasmon resonance in the near infrared can be used to optically detect H2 and NO2 at near to room temperature conditions. Gallium doped zinc oxide (GZO) and silicon doped zinc oxide (SZO) nanocrystals with a tunable surface plasmon resonance peak in the near infrared are obtained using a non aqueous colloidal heat-up synthesis. Thanks to the strong sensitivity of the of the plasmon resonances to chemical or electrical changes occurring at the surface of the nanocrystals, such optical features can be used to detect toxic gases. We demonstrate that both GZO and SZO thin films prepared depositing an assembly of highly doped ZnO colloids are able to optically detect both oxidizing and reducing gases. Combined optical and electrical measurements show that trivalent dopants within ZnO nanocrystals enhance the gas sensing response compared to undoped ZnO. Moreover, light irradiation is used to increase the performance of the sensor and reduce drastically the operative temperature. These plasmonic infrared sensors based on degenerately doped semiconductors represent a marked advancement towards achieving highly sensitive and selective sensors.

12:00 CMOS integrated metal oxide nanowire devices for environmental sensing **X.III.6**

Authors : Anton Koeck, Johanna Krainer, Eva Lackner, Florentyna Sosada, Robert Wimmer-Teubenbacher, Stephan Steinhauer, Karl Rohracher, Ewald Wachmann, Martin Schrems
Affiliations : Materials for Microelectronics, Materials Center

Leoben Forschung GmbH, Roseggerstrasse 12, 8700 Leoben, Austria; Okinawa Institute of Science and Technology (OIST) Graduate University, 1919-1 Onna-Son, Okinawa 904-0495, Japan; ams AG, Tobelbaderstrasse 30, 8141 Unterpremstaetten, Austria

Resume : Gas sensors are of high importance for many applications ranging from indoor air quality monitoring and personal safety systems to outdoor environmental monitoring. The employment of metal oxide nanowires is a very powerful strategy to push the performance of gas sensing devices. Nanowire integration with standard CMOS technology, however, remains a major challenge. We present electronic gas sensor devices based on different types of metal oxide nanowires, such as CuO and ZnO nanowires, which are directly synthesized on CMOS fabricated microhotplate (µhp) chips by a thermal oxidation process. Other types, such as SnO2 and WO3 nanowires, are transferred to the µhp chips by a special process technology. The fabrication procedure results in multi-nanowire devices, where many nanowires in parallel are employed as gas sensing components. The µhp chips are fabricated in standard 0.35µm CMOS technology and are designed for Through-Silicon-Via technology to enable 3D-integration to a smart System-in-Package. We will present gas sensor measurements toward different target gases such as CO, CO2, and a specific HC-mix both in dry as well as in humid synthetic air. The presented technologies can be used in a CMOS backend process and enable the fabrication of CMOS integrated metal oxide nanowire gas sensing devices. Such CMOS integrated nanowire arrays are highly promising candidates for realizing smart multi-parameter sensing devices for the consumer market. This work was done within the project “MSP - Multi Sensor Platform for Smart Building Management” (FP7-ICT-2013-10 Collaborative Project, No. 611887).

12:30 *Lunch*

Modelling of Sensors and Sensor/Gas Interaction : Eduard Llobet

14:00 **New Insights into the Sensing Mechanism of Shape Controlled ZnO Particles** **X.IV.1** ☆

Authors : Massimiliano D'Arienzo, Matteo Redaelli, Franca Morazzoni, Barbara Di Credico, Roberto Scotti
Affiliations : University of Milano-Bicocca, Department of Materials Science, via R.Cozzi 55, 20125 Milano, Italy

Resume : The unique properties of shape controlled ZnO particles as gas-sensors have been largely reported. However, a clear assessment of their sensing mechanism is still an open challenge. Aiming to contribute in facing with this issue, we compared the sensing behavior of morphology-controlled ZnO crystals with specific exposed surfaces to that of ZnO (ZnO®) particles with uneven shape. Besides an expected higher electrical response for shape controlled crystals exposing (0001) high-energy surfaces, we observed significant differences in the reactivity of their VO• paramagnetic species. In fact, the ESR spectra of ZnO® revealed that these defects increase upon interaction with CO while decrease under oxidation treatments. In shape controlled crystals an opposite trend has instead been observed. From these outcomes, we have proposed morphology-dependent sensing mechanisms. While in ZnO® irregular nanoparticles the sensing is associated to an oxygen vacancy mechanism, in shape controlled crystals it seems only indirectly involve the oxygen defects. This corroborates the idea, considered valuable in many studies, that the sensing properties of ZnO particles with predominant (0001) surfaces rely on an oxygen ionosorption mechanism. We believe that these findings and the adopted approach may positively contribute to the debate still existing

between the so called “oxygen vacancy” and “ionosorption” models in the interpretation of sensing of semiconductor metal-oxides.

14:15 Single-emitter all-inorganic ratiometric pressure sensitive paints based on dual-emitting dot-in-bulk nanocrystals **X.IV.2**

Authors : Monica Lorenzon (1), Wan Ki Bae (2), Valerio Pinchetti (1), Francesco Meinardi (1), Victor I. Klimov (3), Sergio Brovelli (1).
Affiliations : Monica Lorenzon, Dipartimento di Scienza dei Materiali, Università degli Studi di Milano Bicocca, Milano, Italy; Wan Ki Bae, Korea Institute of Science and Technology, Seoul, Korea (the Republic of); Valerio Pinchetti, Dipartimento di Scienza dei Materiali, Università degli Studi di Milano Bicocca, Milano, Italy; Francesco Meinardi, Dipartimento di Scienza dei Materiali, Università degli Studi di Milano Bicocca, Milano, Italy; Victor I. Klimov, Chemistry Division and Center for Advanced Solar Photophysics, Los Alamos National Laboratory, Los Alamos, New Mexico, United States; Sergio Brovelli, Dipartimento di Scienza dei Materiali, Università degli Studi di Milano Bicocca, Milano, Italy

Resume : Pressure sensitive paints (PSPs) are effective, non-intrusive tools used to map the O2 flow on complex surfaces through simple optical detection. Their functioning mechanism relies on the photoluminescence (PL) quenching experienced by suitable chromophores exposed to O2. Quantitative O2 detection, however, requires sophisticated calibration protocols to correct for experimental geometry and temperature. Ratiometric PSPs (rPSPs) can overcome this limits exploiting the different sensitivity to O2 of coexisting emissive states. To date, all reported rPSPs are based on mixtures of organic chromophores or dye-functionalized nanocrystals (NCs), which suffer from phase segregation, energy transfer and different temperature sensitivities of the emitters. Here, we report the first example of rPSPs based on a single type of emitter, namely CdSe NCs coated with ultra-thick CdS shells exhibiting dual-color PL arising from simultaneous radiative recombination of core- and shell-localized excitons. Since red-emitting core excitons are separated from the environment by the shell, they are unaffected by O2 that instead severely quenches the green shell PL1. As a result, upon lowering the O2 pressure from 1 to 10-3 bar, the green PL undergoes >300% increase, whereas the core PL remains largely unvaried, with the total emission color changing from red to yellow to green. This result confirms their suitability for a disruptive advancement in the field of rPSPs. 1 NanoLett 2014, 14, (7), 3855.

14:30 Hybrid phenyl-silica xerogel films to detect volatile organic compounds. Determination of the molar enthalpy of adsorption **X.IV.3**

Authors : Calleja, I., Echeverría, J.C., Moriones, P., Garrido, J.J.
Affiliations : Departamento de Química Aplicada. Universidad Pública de Navarra. Campus Arrosadía, 31006 Pamplona. Spain.

Resume : Fiber-optic sensors (FOS) based on porous silica films that operate in reflectance mode are very suitable to detect volatile organic compounds (VOCs). These sensors combine the advantages of the optical fiber with the flexibility of the sol-gel process to obtain silica films with controlled porous texture and surface chemistry. We report experimental results on the effect of temperature (15 – 50 ºC) on the response of FOS that use films of phenyl-silica xerogels as the sensing elements. The sols were prepared by the sol-gel process at pH

10 with mixtures of Phenyltriethoxysilane (PhTEOS) and Tetraethylorthosilane (TEOS) in 30:70, 40:60, and 50:50 molar percentages. Films were affixed to the end of the optical fiber by the dip-coating technique. The measuring system works under volumetric static conditions. FTIR and 29Si-NMR spectroscopies confirmed the presence of Si-C bonds and that the phenyl group was incorporated into the xerogels. The response decreased with temperature, which can be attributed to the decrease in the adsorption of VOCs. At a given temperature, experimental data agreed with a model based on adsorption of VOCs molecules on the film that, in turn, changes the refractive index of the external medium. Applying the Clausius-Clapeyron equation to the experimental data at different temperatures provided the molar enthalpy of adsorption, which for n-hexane varied from 11 to 36 kJ mol-1.

14:45 Photonic Crystals for Gas Sensing: Hydrogen Measurements with Tungsten Oxide Inverse Opals **X.IV.4** ☆

Authors : Sabrina Amrehn, Simon Vetter, Thorsten Wagner
Affiliations : University of Paderborn

Resume : We present a new concept for gas sensing with an optical read out. Hydrogen measurements based on a tungsten oxide inverse opal with contactless signal detection were investigated. This approach allows us to quantify hydrogen under harsh conditions. The chosen material design leads to the optical properties, which allow the optical read out of a known gas reaction between tungsten oxide and hydrogen. The sensor setup is based on photonic crystals, which were synthesized in an easy way using a casting method. The reflectance spectrum of such crystals is mainly defined by the periodicity of the two materials it consists of and their refractive indices. During the gas reaction the refractive index of the tungsten oxide changes and so the reflectance spectrum of the crystal is manipulated. This allows us to use the shift of the reflectance maximum as a sensor signal with contactless optical read out. Besides measurements we also present a model and simulations of how the sensing mechanism might work.

15:00 Conductivity and gas sensing mechanism of nanocrystalline TiO2 – SnO2 – a review **X.IV.5** ☆

Authors : K. Zakrzewska (a), M. Rekas (b), M. Radecka (b)
Affiliations : (a) Faculty of Computer Science, Electronics and Telecommunications, AGH University of Science and Technology, al. A. Mickiewicza 30, Krakow 30-059, Poland; (b) Faculty of Materials Science and Ceramics, AGH University of Science and Technology, al. A. Mickiewicza 30, Krakow 30-059, Poland

Resume : The aim of this work is to present a review on the conductivity and gas sensing mechanism nanocomposites of TiO2 – SnO2 as compared with solid solutions and microcrystalline thin films. Mixed-oxide system of TiO2-SnO2 is believed to be an efficient active material for gas sensing resistors with improved selectivity. Chung et al [1] were the first to report on stable CH4 and CO sensors of this type in 1992. It has been suggested [1] that the improved gas sensing performance relies on the Schottky barrier formation at grain boundaries of well-developed SnO2 grains embedded in the finely dispersed TiO2 amorphous matrix. Since then, numerous papers appeared [2-4] among which our own contributions [5-8] dealing with different forms of TiO2-SnO2 system. We have studied gas sensing and catalytic behavior of microcrystalline ceramics, thin films and quite recently the nanomaterials. The

motivation for these investigations relies in the unresolved problem whether the simple mixture of constituents or the solid solution demonstrates better sensing properties. This work presents a survey of the research carried out for TiO2-SnO2 materials in order to compare their properties in the case of composites and solid solutions. References [1] Chung WY, Lee DD, Sohn BK. Effects of added TiO2 on the characteristics of SnO2-based thick film gas sensors, Thin Solid Films 1992;221:304-309. [2] Dusastre V, Williams DE. Gas-sensitive resistor properties of the solid solution series Tix(Sn1-ySby)1-xO2 (0

15:30 *Coffee break*

Carbon Nanomaterials for Chemical Detection : Mohamed Saad

16:00 **Carbon-based hybrid materials for the development of sensor-systems dedicated to environmental gaseous pollutants** **X.V.1**

Authors : Jérôme BRUNET, Alain PAULY, Amadou NDIAYE
Affiliations : Clermont Université, Université Blaise Pascal, Institut Pascal, BP 10448, F-63000 Clermont-Ferrand, France; CNRS, UMR 6602, Institut Pascal, F-63178 Aubière, France

Resume : The emergence of nanocarbonaceous materials has enabled a real advance on the development of new functional materials especially in the field of chemical sensors. If their aromatic nature and the modulation of their surface chemistry make possible their functionalization by covalent or non-covalent bonding of functional groups, the high specific surface area of nanocarbons ensure the distribution of sensing molecules onto a large surface. Thus, a large number of actives sites can interact with the target analytes, leading to sensing devices with higher sensitivity, lower detection level and high resolution. Such performances are key factors for sensors devoted to environmental monitoring. Original hybrid materials have been developed based on the non-covalent functionalization of nanocarbons by indigo or metallophthalocyanine organic molecules. The non-covalent functionalization of nanocarbons have been emphasized by SEM, TEM, XRD and TGA characterizations. The interactions of aromatic hydrocarbons on phthalocyanine/nanocarbons materials have been exploited for the development of QCM-based sensors devoted to benzene, toluene and xylene detection à room temperature. Complementary, the irreversible chemisorption of ozone on indigo/nanocarbons hybrid material led to the achievement of selective filters with high durability. Associated to phthalocyanine chemoresistor into a sensor-system, such filter enable the selective measurement of nitrogen dioxide at ppb level in air.

16:30 **Fabrication of hydrogen gas sensor using single walled carbon nanohorn based hybrid nanostructure** **X.V.2**

Authors : Shivani Dhall and B.R. Mehta
Affiliations : Department of Physics, Indian Institute of Technology, Delhi-110016, India.

Resume : Cost effective and quick detection of hydrogen gas at room temperature has always remained a challenge. This study reports the hydrogen gas sensing characterstics of hybrid nanostructure using single walled carbon nanohorn (SWCNHs) fabricated by simple chemical method. The sensing response of hybrid nanostructure is due to their change in electronic nature structure on the exposure of H2 gas and this are important for understanding the effect of gas adsorption on their electronic conduction. In addition, the sensor fabrication involves simply drop-casting treatment at room temperature in

normal condition. The repeatability and low recovery time in N2 atmosphere of this sensor are the main advantages for the detection of low concentration (2%) of H2 gas at the room temperature conditions.

16:45 **Mesoporous nitrogen containing carbon for highly sensitive electrochemical detection of heavy metals** **X.V.3**

Authors : Anju Joshi* and Tharamani C. Nagaiah
Affiliations : Department of Chemistry, Indian Institute of Technology Ropar, Rupnagar, Punjab 140 001, India

Resume : Mesoporous nitrogen rich carbon (MNC) material has been prepared as a highly sensitive and conveniently usable probe for electrochemical determination of heavy metal ions including Pb (II), Cd (II) and Cu (II). Spontaneous adsorbability of MNC material has been utilized for eliminating the requirement of pre-concentration step, essentially involved in determination of metal ions. Square wave stripping voltammetry (SWSV) studies implied the superior electrocatalytic activity of MNC modified GCE (MNC/GCE) towards determination of Pb (II) and Cd (II). The linear calibration curves range from 0.01 µM-100 µM and 0.01 µM-70 µM for simultaneous determination of Cd(II) and Pb(II) with an excellent sensitivity of 18.46 µA µM-1 cm-2 and 87.71 µA µM-1 cm-2 respectively. The limit of detection (LOD) for simultaneous determination of Pb (II) and Cd (II) was calculated out to be 0.0005 µM and 0.001 µM (3σ method) which suggests the potential efficacy of MNC towards continuous monitoring of Pb (II) and Cd (II) in natural water resources without requirement of time-consuming pre-concentration step.

17:00 **The role of surface chemistry in functionalized CNTs-based gas sensors: material design and application to atmospheric pollutant** **X.V.4**

Authors : A. L. Ndiaye (1,2), J. Brunet (1,2), C. Varenne (1,2), A. Pauly (1,2)
Affiliations : (1) Clermont Université, Université Blaise Pascal, Institut Pascal, BP 10448, F-63000 Clermont-Ferrand, (2) CNRS, UMR 6602, Institut Pascal, F-63178 Aubière

Resume : As member of the wide family of carbon materials, the carbon nanotubes (CNTs) offer remarkable properties [1] which are closely related to their narrow structure and surface chemistry. For gas sensors where matrices of higher surface area are potentially appealing, carbon nanotubes are good candidates to fulfil efficient gas sensors requirement. Additionally, they present electronic and optical properties combined with their suitability for different deposition techniques, and this enables them to be associated to different transduction modes (resistive, electrochemical, mass and optical). These features as well as their versatile surface chemistry make them ideal for developing novel and efficient gas sensors. However, CNTs need to be chemically or physically modified to overcome their lack of solubility and selectivity of detection. To this aim, surface functionalization (covalent and non-covalent) is an excellent option which improved simultaneously the solubility and the selectivity depending on the functional groups attached to the surface. In this context, we have developed sensitive materials based on functionalized CNTs for application devoted to air pollutants monitoring. The prepared sensing materials are characterized by standard techniques (UV-Vis spectroscopy, TGA, TEM, Raman analysis) and sensor responses were established by means of resistive and QCM (Quartz Crystal Microbalance) transducers. References: [1] D.M. Guldi, et. al., Chem. Rev. 2010, 110, 6768.

17:15 Gas sensing properties of MWCNTs layers electrodecorated with Au and Pd nanoparticles **X.V.5**

Authors : Elena Dilonardo,1,2 Michele Penza,3 Marco Alvisi,3 Riccardo Rossi,3 Gennaro Cassano,3 Cinzia Di Franco,4 Francesco Palmisano,1 Luisa Torsi,1 Nicola Cioffi1
Affiliations : 1Department of Chemistry, Università degli Studi di Bari Aldo Moro, Bari, Italy; 2Department of Electrotechnics and Electronics, Politecnico di Bari, Bari, Italy; 3Italian National Agency for New Technologies, Energy and Sustainable Economic Development (ENEA), Department for Sustainability - Lab Functional Materials and Technologies for Sustainable Applications - Brindisi, Italy; 4CNR-IFN Bari, Bari, Italy.

Resume : The preparation and characterization of MWCNTs-based chemiresistors, functionalized with Au and Pd NPs, to improve the sub-ppm detection of gaseous pollutants, compared to pristine ones, is reported. An electrophoretic process was proposed to deposit, directly on the outer MWCNTs sidewalls, electrochemically-preformed Au or Pd NPs with controlled size.[1,2] Different deposition times were used to tune the metal content on MWCNTs, as revealed by chemical and morphological analyses. The gas sensing properties of pristine and doped MWCNTs were evaluated at different operating temperatures (100-200°C) towards various concentrations of gaseous pollutants (e.g. NO2, H2S), and related to the metal used in the doping, and to its loading. Metal-doped MWCNTs sensors exhibited a very high gas sensitivity, fast response, reversibility, good repeatability, and sub-ppm range detection limit, with the MWCNTs sensing properties controlled by the type and loading of used catalyst. Specifically, Au-decorated MWCNTs with the lowest Au content revealed the highest sensitivity towards NO2 at 150°C;[1,2] instead, MWCNTs with the highest Pd loading showed the highest NO2 sensitivity at 100°C. Finally, on the basis of the gas sensing performance of prepared hybrid gas sensors, sensing mechanisms have been proposed, evaluating the effect of their chemical composition. [1] E. Dilonardo et al., Sens. Act. B 2016, 223, 417–428. [2] E. Dilonardo et al., J. Sens. Sens. Syst. 2014, 3, 1–8.

17:30 Novel Pt-free Micro- and nano-structured carbon materials with electrocatalytic activity in oxygen reduction reactions **X.V.6**

Authors : Stefania Marzorati, Serban N. Stamatin, Joana Vasconcelos, Roman Ivanov, Mariangela Longhi, Irina Hussainova, Paula E. Colavita
Affiliations : School of Chemistry and Centre for Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN), University of Dublin Trinity College, College Green, Dublin, Dublin D2, Ireland; Università degli Studi di Milano, Dipartimento di Chimica, Via Golgi 19, 20133 Milano, Italy; Tallinn University of Technology, Ehitajate 5, 19180 Tallinn, Estonia

Resume : Oxygen electrochemistry plays a crucial role in the deployment and large scale adoption of fuel cell (FC) technologies. Some of the most promising FCs in terms of potential to mitigate emissions, rely on the use of Pt-group metals (PGM) as electroctalysts, where most of the metal load is necessary to improve the rate at which the sluggish oxygen reduction reaction (ORR) takes place at the cathode. PGM cost and scarcity have been identified in fact as primary obstacles to large scale applications of FCs; thus, there is great interest in the discovery and optimization of ORR electrocatalysts that do not rely on PGM. N-doped carbons, often in combination with low cost metals, have been shown to display electrocatalytic activity in ORR. In this presentation we will discuss studies of ORR activity of nanostructured N-doped

carbons in the absence and in the presence of non-precious metals in their structure. First, we report on the template-free synthesis via ultrasonic spray pyrolysis of Fe- and N-doped porous carbon microspheres. Scanning Electron Microscopy (SEM), Energy Dispersive Spectroscopy (EDS) and Focused Ion Beam (FIB) milling were used to understand microsphere structure, whereas X-ray Diffraction (XRD) and Photoelectron Spectroscopy (XPS) were used to investigate bulk and surface chemistry. Microspheres were found to display ORR activity in acidic solution; results suggests that direct formation of H2O is the preferred ORR mechanism. Second, we discuss studies of ORR activity in alkaline solution of graphene-like nanostructured carbon with tailored edge-plane density. Interestingly, these materials offer a versatile platform for mechanistic studies of structural and chemical motifs that result in ORR activity in nanocarbons.

17:45 INKJET PRINTED GRAPHENE-BASED CHEMIRESISTIVE SENSORS **X.V.7**

Authors : T. Polichetti1, F. Villani1, F. Loffredo1, C. Schiattarella2, B. Alfano1, M. L. Miglietta1, E. Massera1, G. Di Francia1
Affiliations : 1 ENEA - R.C. Portici, Piazzale E. Fermi 1, Portici (Naples), I-80055, Italy; 2 Department of Physics, University of Naples 'Federico II', Via Cinthia, I-80126, Naples, Italy

Resume : In the recent years, the potential of graphene for sensing applications is widely attracting the interest scientific community on exploiting its outstanding properties. The Liquid Phase Exfoliation (LPE) method is very promising to fabricate graphene-based inks to be deposited by printing techniques. Among them, the inkjet printing (IJP) technology allows to selectively depose small ink volumes in controlled way, reducing the waste materials. Additionally, IJP depositions are no-vacuum, no-temperature and contactless resulting totally versatile for the employable inks and substrates. In the current work, IJP is presented as potential technology to realize reproducible LPE graphene-based chemiresistors and as a sustainable processing method to manufacture sensing device by a green approach, namely by using eco-friendly solvents and recyclable substrates. Two series of sensor devices have been fabricated. In the first case a suspension of graphene obtained by exfoliation of graphite in N-Methyl-2-pyrrolidone solvent has been printed onto Al2O3 substrate. In the second series, according to an ecosustainable approach, the ink was a suspension of graphene in a mixture of isopropanol and ultrapure water printed onto glossy paper. To investigate the device performances, the conductance variations ΔG/G0 have been measured upon exposure to different concentrations of the analytes NO2 and NH3. The tests confirmed the good specificity of pristine graphene towards NO2 with respect to NH3.

18:00 ELECTROCHEMICAL SENSOR BASED ON GOLD NANOPARTICLES-POROUS CARBON NANOCOMPOSITE FOR THE DETERMINATION OF MERCURY **X.V.8**

Authors : Laura Asturias-Arribas (1), Pengfei Niu (1), Martí Gich (1), César Fernández-Sánchez (2), Anna Roig (1)
Affiliations : 1) Institute of Material Science of Barcelona (ICMAB-CSIC), UAB Campus, 08193 Bellaterra, Spain 2) Institute of Microelectronics of Barcelona (CNM-CSIC), UAB Campus, 08193 Bellaterra, Spain

Resume : Mercury has been extensively used in many applications such as light bulbs, measuring instruments or even industrial manufacture of chemical compounds. Its main limitation is its high toxicity, threatening human health and the

environment. Even if an organism is not exposed to high quantities of mercury, low doses can be accumulated in the body, resulting in health problems [1]. That is the reason why mercury is listed as a priority and hazardous substance in the field of water policy by the 2013/39/EU Directive [2]. Therefore, the determination of mercury and its quantification is a very important issue. Standard and traditional analytical techniques used for the analysis of this metal, such as atomic absorption spectroscopy and atomic fluorescence spectrometry, inductively-coupled plasma-mass spectrometry, optical emission spectroscopy and X-ray fluorescence spectrometry, are costly and require specialized staff. Consequently, simple, rapid and low cost techniques that can be deployed on-site providing real-time quantitative results, such as electrochemical sensors, are being developed [3]. Taking into account the properties of porous carbon materials [4] and gold, which has a high affinity for mercury and allows enhancing the pre-concentration of the metal on the electrode [5]; a carbon-gold nanoparticle composite was synthesized by sol-gel chemistry and used in conventional paste electrodes as well as in screen-printed electrodes for the electrochemical determination of mercury in waters. [1] Martín-Yerga, D. et al. Talanta 116 (2013) 1092-1104 [2] Commission Directive 2013/39/EC, Official Journal of European Union, L226/1-17, 24.8.2013. [3] Duarte, K. et al. Trends in Analytical Chemistry 64 (2015) 183-190 [4] Gich, M. et al. Journal of Materials Chemistry A 1 (2013) 11410-11418 [5] Gao, C. et al. Trends in Analytical Chemistry 51 (2013) 1-12

START AT	SUBJECT	View All	NUM.	ADD

Graphene-based Chemical Sensors : Naureen Akhtar

09:00 **2D-Materials on Silicon Carbide as a Platform for Highly Sensitive and Selective Gas Sensors** **X.VI.1**

Authors : J. Eriksson1, R. Yakimova1,2, A. Lloyd Spetz1
Affiliations : 1 Division of Applied Sensor Science, Department of Physics, Chemistry, and Biology, Linköping University, SE-58183, Sweden; 2 Graphensic AB, SE-58333 Linköping, Sweden

Resume : 2D materials offer a unique platform for sensing with extremely high sensitivity, since even minimal chemical interaction causes noticeable changes in electrical conductivity, which can be used as sensor readout. However, the sensitivity has to be complemented with selectivity, and, for many applications, improved response- and recovery times. This has been addressed, for example, by combining graphene (for sensitivity) with metal/oxide nanoparticles (for selectivity). On the other hand, functionalization or modification of the graphene often results in poor reproducibility. Here, we investigate the gas sensing performance of epitaxial graphene on Silicon Carbide (SiC) decorated with nanostructured metallic layers as well as metal-oxide nanoparticles deposited using scalable thin-film deposition techniques, like hollow-cathode pulsed plasma sputtering. Under certain modification conditions the electronic properties of the surface remain those of graphene, while surface chemistry can be tuned to improve sensitivity, selectivity and speed of response to gases relevant for air quality monitoring and control, such as nitrogen dioxide, benzene, and formaldehyde. The presentation will also include results on other monolayer gas sensing layers like iron oxide on top of platinum and 2D metals on SiC, which offer additional possibilities like

operation at high temperature and in harsh conditions, while maintaining all the promises of 2D materials as extremely sensitive transducers.

09:30 **Graphene oxide for sensing applications: investigation of electrical properties and correlation with oxygen functionalities** **X.VI.2**

Authors : S. Scalese 1, S. Baldo 12, D. D'Angelo 1, S. Filice 13, C. Bongiorno 1, I. Deretzis 1, A. La Magna 1
Affiliations : 1 - CNR-IMM, Ottava Strada n.5, I-95121, Catania (Italy); 2 - Dipartimento di Fisica e Astronomia, via S. Sofia n.64, I-95123 Catania (Italy); 3 - Dipartimento di Scienze Chimiche, Università degli Studi di Catania, viale Andrea Doria 6, I-95125 Catania (Italy);

Resume : Graphene-based materials are among the most innovative and promising materials for the development of high-performance sensing devices, mainly due to the large surface area and the possibility to modify its reactivity by suitable functionalization. In the field of sensing applications, the peculiarities of innovative materials can be exploited only if chemical and physical properties are fully understood and correlated to each other. To this aim in this work graphene oxide (GO) and thermally treated GO were investigated from electrical, chemical and structural points of view. GO was deposited between two electrodes by dielectrophoresis, a very cheap and flexible technique that allows to deposit nanostructures with a very good position control and at room temperature. The GO electrical conductivity was investigated by changing the temperature during the characterization: an increase of the conductivity was observed when the device is cooled down and this effect is reversible with the temperature. The opposite trend was observed for thermally treated GO. The effect of different thermal treatments (i.e. temperatures and environment), was investigated and electron energy loss spectroscopy , with the analysis of the multi peaks features of the carbon and oxygen K-edges, allowed to distinguish the different oxygen functionalities preserved after each thermal treatment and to correlate the conduction mechanisms to the chemical and structural properties of the material.

09:45 **Laser deposition on graphene – a versatile method for developing environmental sensors** **X.VI.3**

Authors : Margus Kodu, Artjom Berholts, Tauno Kahro, Markus Veinla, Tea Avarmaa, Ahti Niilisk, Harry Alles, Raivo Jaaniso
Affiliations : Institute of Physics, University of Tartu, Ravila 14c, 50411, Tartu, Estonia

Resume : Graphene as 2D material can be fully exposed to environment and hence provides an ideal platform for chemical sensing. However, in order to achieve the sensitivity and selectivity required by environmental sensors, additional adsorption centres have to be created at its surface e.g. by controlled formation of defects, dopants or clusters. In the present work, we demonstrate the functionalization of single layer graphene by pulsed laser deposition (PLD) and its impact on the sensitivity to main pollutant gases. PLD can be used as a precise tailoring tool for this purpose as typically only ~1/100th of a monolayer is deposited by a single laser pulse. The dependence of gas sensitivity and response speed from the composition and amount of deposited material as well as from its average 'landing energy' on graphene was studied. Different target materials were used for functionalizing graphene: metals (Ag, Pd, Ru, Au), oxides (ZrO_2, SnO_2, TiO_2, NiO), nitride (TiN). Average thickness of deposited material was varied between 0.01 to 20

monolayers. The surface morphology of deposited materials and defectiveness of graphene were studied. Performance benchmarking with commercial semiconductor NO2 sensors showed that the sensitivity of our graphene-based sensors was in the practical range and such figures of merit as the sensitivity divided by long-term drift or by cross-sensitivity to humidity were superior in case of graphene based sensors.

10:00 *Coffee break*

Catalytic Materials for Environmental Sensing : Anton Köck

10:30 **Laser shaped thick-film IDE for nanoparticle detection at high frequencies.** **X.VII.1**

Authors : Maciej Sobocinski1, Sami Myllymäki1, Mikko Nelo1, Mike Andersson1,2, Jari Juuti1, Joni Kilpijärvi1, Niina Halonen1, Tuomo Siponkoski1, Heli Jantunen1, Anita Lloyd Spetz1,2
Affiliations : 1. Microelectronics and Materials Physics Laboratories, University of Oulu, P.O. Box 4500, FI-90014 University of Oulu, Finland 2. Division of Applied Sensor Science, Department of Physics, Chemistry and Biology, Linköping University, SE-58183 Linköping, Sweden

Resume : Growing awareness about impact of pollution for human health, development of industry, and growing use of nanomaterials, has increased the need for monitoring of air quality. Nano size dust and ash particles can pose serious health issues. Moreover, certain technologies such as microelectronics and pharmacology require dust free environments. Several Particulate Matter (PM) sensors have already been developed, however there is a need to detect smaller particles and smaller concentrations as well as increasing the portability of the devices and shorten the time of analysis. In this paper, laser shaped thick-film interdigitated electrodes are used for capacitive sensing of nanoparticles at high frequencies. The sensors have been manufactured in Low Temperature Co-fired Ceramic, which is a well-established packaging technology offering many advantages such as cost-effectiveness resistance to high temperatures and harsh environments. Different designs were tested and sensitivity test was performed for chosen designs. Sensors were exposed to two different nanoparticles, 40 nm CuO and 8-11 nm carbon black using ink-jet printing as a method to provide controlled amount of nanoparticles on selected area. The sensor signals were measured at 1 GHz to 10 GHz providing clear responses for both nanoparticles compared to reference signal without particles. Thus, high frequency based detection of nanoparticles with thick-film IDE structure appears promising for nanoparticle detection.

11:00 **Design process of an autonomous–operating hydrogen sensor using nanostructured Palladium Platinum and Surface Acoustic Wave** **X.VII.2**

Authors : Leonardo Perez-Cortes, Camilo Hernandez-Rodríguez, Thomas Mazingue, Marc Lomello-Tafin
Affiliations : Université Savoie Mont Blanc, Laboratoire SYMME.

Resume : Actual hydrogen (H2) sensors require high sensitivity, autonomous operation and easy integration in fuel cell technologies for stationary and portable power. This article presents the design process of an innovative Surface Acoustic Wave hydrogen sensor based on a Palladium-Platinum (PdPt) catalytic material developed in a previous research. Among the advantages of this sensor there are

wireless data accessibility without the need of any power supply. Under H2 exposure, the nanostructured PdPt catalyst exhibits repeatable and reversible exothermal response, such that its temperature is correlated with H2 concentration (2°C in 4000 ppm of H2). The sensing is carried out by a SAW transducer which transforms the PdPt temperature variations derived from the catalytic reaction into an electrical signal relative to the H2 concentration. Our design process allows to develop an optimal sensor system including the electrical and mechanical structure, for high sensitivity applications.

11:15 Recognition abilities of nano-tweezers based on polyoxometalates bis-functionalized with organic chromophores **X.VII.3**

Authors : Marcella Bonchio, Mauro Carraro
Affiliations : University of Padova - Department of Chemical Sciences and ITM-CNR, Via Marzolo 1, 35131, Padova, Italy

Resume : Hybrid organic-inorganic molecular species can be very appealing for the development of novel nanodevices for sensing and energy conversion. Divacant polyoxometalates (POM) are robust and molecular polyanionic metal-oxides that can be conveniently exploited as inorganic platforms for anchoring two organic pendants in a tweezer-type arrangement. In particular, the use of organic chromophores as pendants enables the use of spectrophotometric and spectrofluorimetric techniques to highlight recognition phenomena of metal ions and organic molecules, involving an interplay of the two domains. Recent results obtained with different hybrid POMs, including complexes bis-functionalized with pyrene or dansyl moieties will be presented, demonstrating the possibility to use these nano-sized hybrids for sensing applications (with metal ions) and for the preparation of ordered materials (upon interaction with carbon nanostructures).

11:30 Polymer and co-Polymer Caoted Quartz Crystal Microbalance for Volatile Organic Compounds Detection at Room Temperature **X.VII.4**

Authors : Sadullah Öztürk1*, Derya Malkoç1, Arif Kösemen2, 3, Zafer Şen4, Necmettin Kılınç5, Mika Harbeck4, Zafer Ziya Öztürk2
Affiliations : 1Fatih Sultan Mehmet Vakif University, Faculty of Engineering, 34080, Istanbul, Turkey; 2Gebze Institute of Technology, Science Faculty, Department of Physics, 41400, Gebze-Kocaeli, Turkey; 3 Mus Alparslan University, Department of Physics, 49100 Mus, Turkey; 4 TUBİTAK-MAM, 41470 Gebze, Kocaeli, Turkey; 5Nigde University, Faculty of Engineering, Mechatronics Engineering Department and Nanotechnology, Application & Research Center, Nigde University, 51245 Nigde, Turkey, 51245 Nigde, Turkey

Resume : In this study, polythiophene and polythiol were deposited onto the mass sensitive transducer is quartz crystal microbalance (QCM) to detect volatile organic compounds at room temperature. Fabricated samples were tested to VOCs by using home-made gas sensing set up. Test concentrations of the volatile organic compounds were calculated using vapor pressure at constant temperature using Antonio equations. Moreover, all fabricated sensors have good sensor characteristic as reliable, durable and also recovery even one month later. On the other hand sensing mechanism and surface interactions between actual VOCs and sensitive materials surface were investigated.

Acknowledgement: This study was supported by The Scientific and Technological Research Council of Turkey (TUBITAK) Grant No: 113F403

11:45

High sensitivity and low operating temperature acetone sensors based on ZnO:Au and ZnO:Pd compounds

X.VII.5

Authors : Melina Alexiadou, Maria Kandyla, Michael Kompitsas
Affiliations : Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation

Resume : Acetone, the most commonly used solvent in research and industry, is highly volatile and hazardous to human health and living organisms. Exposure to high concentrations of acetone vapor may cause headache, allergy, fatigue, and even narcosis. Acetone contained in the human breath is an indicator of blood glucose levels. Hence sensitive detection and quantification of acetone is essential. In this study, acetone sensors based on ZnO:Au and ZnO:Pd compounds were developed. Zinc oxide thin films were grown by pulsed laser deposition (PLD) and nanopatricles of gold or palladium were subsequently laser-deposited on the surface of the ZnO films. The ZnO:Au and ZnO:Pd films were tested as acetone sensors. We find that the presence of the Au or Pd nanoparticles improves the detection of acetone. As the quantity of metallic nanoparticles on the ZnO surface increases, the operating temperature, for which small concentrations of acetone are detected, decreases. The operating temperature of the sensors was 155 – 200 0C, which leads to lower power consumption and increased operating safety, compared to other metal oxide acetone sensors which operate at higher temperatures. The response time of the sensors decreased for thicker ZnO films. The ZnO:Pd compound performed better as an acetone sensor.

12:00

Under-Water Superoleophobic Sapphire (0001) Surfaces

X.VII.6

Authors : Naureen Akhtar, Vårin R. A. Holm, Peter J. Thomas, Benny Svardal, Simen H. Askeland, and Bodil Holst
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Resume : Owing to its excellent mechanical and thermal properties as well as optical performance, sapphire (crystalline Al2O3, alpha alumina) is extensively used as window in optical sensors for harsh conditions, for example underwater surveillance in the oil industry. However, under these conditions the sapphire surfaces are continuously exposed to oil and other fouling mixtures, which can lead to contamination of the window surface. Hence, making the surface underwater oleophobic would be highly desirable. We found out that a sapphire surface can change from oleophilic to superoleophobic depending on the crystal miscut, polishing method and initial cleanliness state when submerged in water. Moreover, giving the surface the hydrophilic character improves the underwater oleophobic character. This could be understood in the context of underwater superoleophobic surfaces found in nature that exhibit higher propensity for trapping water. Inspired by the underwater superoleophobic self-cleaning surfaces found in nature such as fish scales, sapphire surfaces could be further developed for maintenance free solutions for permanent underwater installation of optical instrumentation.

12:30 *Lunch*

Poster Session II - Materials for Energy Systems and Devices : Anita Lloyd Spetz and Michele Penza

14:00 **Electrodeposited Ag2S onto porous TiO2 thin films for semiconductor-sensitized photocatalytic and photoelectrochemical** **X.PII.1**

Authors : Ibtissem Ben Assaker*; Aymen Bourezgui; Jamila Ben Naceur; Mounir Gannouni; Radhouane Chtourou
Affiliations : Laboratoire Photovoltaïque, Centre de Recherches et des Technologies de l'Energie Technopole borj cedria, Bp 95, hammamm lif 2050, Tunisie

Resume : Much attention has been paid to water splitting process by light irradiation because of its potential to obtain clean and high energy from water [1]. Among variety of materials, TiO2 has drawn much attention because of its promising applications in utilization of solar energy such as photocatalysis [2], photovoltaic [2] and photocatalytic water splitting [4]. To improve these properties, the morphologies and macroscopic structures of TiO2have been intensively studied by many authors in the literature [5]. Moreover, the synthesis of porous structures has attracted increasing interest of researchers [6] as their potential applications in the field of catalysis, ion exchange, and adsorption. Various strategies were taken into account regarding this sphere of study. Latex spheres can be used as templates to form ordered macroporous materials [7]. Despite these efforts, the photocatalytic performance of porous TiO2 was restricted by its low visible light absorption and its fast recombination of photo-generated electrons and holes. Therefore to enlarge the photoresponse spectrum, considerable efforts have been made, such as doping with transition and/or noble metals, non-metals, deposition in quantum dots and construction of heterojunctions with other semiconductors. Construction of a heterojunction between porous TiO2 and other semiconductors with a suitable band gap is an effective method to extend the light absorption spectrum and accelerate photogenerated electron-hole separation, thus enhancing the solar-to-hydrogen conversion efficiency [8]. Silver Sulfide (Ag2S) is a binary chalcogenide semiconductor with a narrow band gap well corresponding to the visible spectrum and considerable photostability in aqueous solution under light irradiation. Several methods have been used for the synthesis of various nanostructures of Ag2S such as nanosheet, nanowire and microsphere for solar water splitting. Among these approaches, electrodeposition technique [9] was used for the deposition of Ag2S thin films onto TiO2. Compared with other deposition methods, electrodeposition provide numerous advantages, including, low temperature processing, arbitrary substrate shapes, controllable film thickness, morphology, and potential low capital cost. It is an isothermal process mainly controlled by electrical parameters. In the present work, semiconducting low band gap Ag2S thin films are used to sensitize highly-oriented porous TiO2 thin films. In this context, we will prepare Ag2S coated TiO2 thin films supported on ITO coated glass combining the sol-gel process, spin coating and electrodeposition technique. This work reports the synthesis conditions, the main physic-chemical characterizations of the resulting hetero-junctions, including X-ray diffraction (XRD), scanning electron microscopy (SEM) and UV-Visible absorption spectroscopy; the photocatalytic activity of Ag2S and heterostructure Ag2S /TiO2 was measured following the degradation of an organic model substrate, methylene blue under visible light. The photoelectrochemical properties of the samples were also studied. References [1] Z. Zou, J. Ye , K. Sayama, H. Arakawa, Direct splitting of water under visible light irradiation with an oxide semiconductor photocatalyst. Nature 7 (2001) 414-625. [2] K. Nakata, T. Ochiai, T.

Murakami, A. Fujishima, Photoenergy conversion with TiO2 photocatalysis , Electrochemica Acta 84 (2012) 103-111. [3] X. J. Huang, Y.K. Choi, Chemical sensors based on nanostructured materials. Sensors Actuators B (2007) 122:659. [4] A. Fujishima, k. Honda, Electrochemical photolysis of water at a semiconductor electrode, Nature 238 (1972) 37. [5] W.J. Yang, C.Y. Hsu, Y.W. Liu, R.Q. Hsu, T.W. Lu, C.C. Hu, The structure and photocatalytic activity of TiO2 thin films deposited by dc magnetron sputtering, Superlattices and Microstructures, Volume 52, Issue 6, December 2012, pp.1131-1142 [6] H. Behera, S. Mandal, T. Sahoo, Oblique wave trapping by porous and flexible structures in a two-layer fluid, Phys Fluids, 25 (11), 2013 [7] Zhiqiang Sun, Yunfeng Li, Yanfang Wang, Xin Chen, Junhu Zhang, Kai Zhang, Zifeng Wang, ChunxiaoBao, JianboZeng, Bing Zhao, and Bai Yang, Three-Dimensional Colloidal Crystal-Assisted Lithography for Two-Dimensional Patterned Arrays, Langmuir, 23 (21), 10725 (2007) [8] C. Han, Z. Li, J. Shen, photocatalytic degradation of dodecyl-benzenesulfonate over TiO2-Cu2O under visible irradiation, Journal of Hazardous Materials 168 (2009) 215-219. [9] Ibtissem Ben Assaker, MounirGannouni, Jamila Ben Naceur, Munirah Abdullah Almessiere, AmalLafy Al-Otaibi, TaherGhrib, ShouwenShen, RadhouaneChtourou , Electrodeposited ZnIn2S4 onto TiO2 thin films for semiconductor-sensitized photocatalytic and photoelectrochemical applications, Applied Surface Science, Volume 351, 1 October 2015, pp. 927-934

14:00 Low sintering with improved performance BaTiO3 piezoelectric ceramics **X.PII.2**

Authors : Rémy Ul, Elodie Leveugle, Mai Pham Thi
Affiliations : Thales Research & Technology Palaiseau France, INSA Blois France ; Thales Research & Technology Palaiseau France ; Thales Research & Technology Palaiseau France

Resume : Lead-free piezoelectric ceramics are urgently needed to replace the PZT-based materials because of their lead oxide toxicity. Ceramics such as BaTiO3 are promising candidate, however the properties of pure BaTiO3 are still very low (d33= 150; kt= 22%) compared with very hard PZT. One way of improvement is the doping with donor and/or acceptor. Thus, Co, Ca and Nb-doped BaTiO3 ceramics were prepared using conventional solid state reaction. The Co3+/Co2+, substituting as donor, leads to oxygen vacancies in ABO3 perovskite structure but increases the piezoelectric performance (d33 = 210 pC/N and kt= 39%). To balance the structural defects, Co substitution with Nb 5+ acceptor or thermal annealing at 1000°C under O2 atmosphere was studied. It improves the properties with d33= 250pC/N and kt= 45%. Furthermore a study of the ceramic process has been made in order to bring it closer to industrial process. The first purpose was to lower the sintering temperature by using Li2O as sintering aid. Thus, addition of Li2O yields dense ceramics with relative density d= 95–98% and with acceptable piezoelectric properties (d33= 210pC/N, kt= 42%) at 1100°C instead of 1350°C as in BaTiO3 conventional sintering. Moreover, the homogeneity of the material has been studied as well as the homogeneity obtained during the ceramic process in the furnace. The microstructure and the properties have been observed and tests have been carried out on 22 samples at the same time.

14:00 Combined experimentaltheoretical study of the optoelectronic properties of non-stoichiometric pyrochlore bismuth titanate **X.PII.3**

Authors : Dalal Noureldine, SheikhaLarchi, Ahmed Ziani, MoussabHarb, Luigi Cavallo, Kazuhiro Takanabe
Affiliations : Division of Physical Sciences and Engineering, KAUST Catalysis Center (KCC), King Abdullah University of Science and Technology (KAUST), 4700 KAUST, Thuwal, Saudi Arabia

Resume : In the light of increasing demands on energy resources, solar energy emerges as a promising alternative to fossil fuels. It is advantageous as it produces clean, renewable, and sustainable forms of energies. Many technologies have been developed to efficiently utilize the sunlight. These include variety of solar cells in addition to using photocatalysis for water splitting reaction. Most of these technologies are based on semiconductors that play the role of light absorbers and/ or charge transporters. In this sense, it is important to characterize the intrinsic properties of the semiconductor and be able to rationalize its efficiency. The Bismuth titanate are interesting family of semiconductors and they have been used in several applications being pigments, photocatalysts, and as ferroelectric material. The pyrochlore structure Bi2Ti2O7 is of particular interest due to its important photo physical properties. However, due to inconsistencies about their crystal structure- being stoichiometric or defected structure, the consequent physical properties are not fully extracted. Therefore we investigate the optoelectronic properties as well as the crystal structure using a combination of experimental and computational methods. Experimentally, the non-stoichiometric Bi2-xTi2O7-1.5x was synthesized both as powder and thin film. The analysis of the crystal structure of the synthesized powders X-ray diffraction spectroscopy (XRD) and the Rietveld refinement showed that the pyrochlore structure adopts the non-stoichiometric Bi2-xTi2O7-1.5xstructure with x ~ 0.25. This agrees with the thermodynamic stability of the defect-containing structure computed using density functional theory (DFT). Intrinsic parameters such as the electronic structure, the effective electron and holemasses, the dielectricconstant, and the absorption coefficient were computed using the density functional perturbation theory (DFPT) approach which was used along with thestandard GGA PBE functional and the screened Coulomb hybrid HSE06 functional, including spinorbitcoupling. An excellent agreement is found between the calculated and measured values for these properties. This supports the overall analysis and opens the door of the bismuth titanate for potential applications as a wide-bandgap material, e.g., as a substitute for TiO2 in dyesensitizedsolar cells and UV-light-driven photocatalysis. This study presents an example of the effective strategy to predict the photo physical properties of semiconductor material.

14:00 One-step hydrothermal synthetic electroactivity POM-MOF for electrocatalysis methanol oxidative **X.PII.4**

Authors : Zhichao Jin,Kaikai Ma,Yanfang Gao(Contact Author)
Affiliations : College of Chemical Engineering;Inner Mongolia University of Technology

Resume : Electrocatalysis oxidative of methanol with CO applied heterogeneous electrocatalyst was studied at normal temperature and pressure.A compound ([Cu2(BTC)4/3(H2O)2]6[H3PW12O40]·(C4H12N)2) was compose by keggin polyoxometalates (POM H3PW12O40) and metal-organic framework (MOF HKUST-1) was synthesized from the simple one-step hydrothermal reaction[1,2]. In this POM-MOF material, the commendable catalytically oxidized active Keggin polyoxometalates was alternately arrayed as noncoordinating guests in the cuboctahedral cages of a Cu-BTC-based metal-organic

framework (MOF) host matrix[2]. The pure bulk POMs present relatively small surface areas (<10m2 g-1) that hinder accessibility to the active sites. Therefore, the applications of POMs as solid catalysts are limited. A self-designed self-fabricated two-compartment electrolytic cell made of polytetrafluoroethylene was constructed for electrocatalysis experiments. The as-synthesized compound POM-MOF showed electrochemically active for methanol[3].
Keywords: electrocatalysis , heterogeneous ,methanol,POM-MOF
[1] Sun, C. Y., Liu, S. X., Liang, D. D., Shao, K. Z., Ren, Y. H., & Su, Z. M. (2009). Highly stable crystalline catalysts based on a microporous metal− organic framework and polyoxometalates. Journal of the American Chemical Society, 131(5), 1883-1888. [2] Song, J., Luo, Z., Britt, D. K., Furukawa, H., Yaghi, O. M., Hardcastle, K. I., & Hill, C. L. (2011). A multiunit catalyst with synergistic stability and reactivity: A polyoxometalate–metal organic framework for aerobic decontamination. Journal of the American Chemical Society, 133(42), 16839-16846. [3] Jia G, Zhang W, Jin Z, et al. Electrocatalytically Active MOF/Graphite Oxide Hybrid for Electrosynthesis of Dimethyl Carbonate[J]. Electrochimica Acta, 2014, 144: 1-6.

14:00

Control of Selective Ion Transportation through Pt film coated PTFE Membrane under Electrical Bias

X.PII.5

Authors : Jeong Hwan Kim, Sun A Jung, Sung Woong Lee, Hyun Jung Yoon, Jae-Sung Yoon, and Yeong-Eun Yoo
Affiliations : Department of Nano Manufacturing Technology, Korea Institute of Machinery and Materials(KIMM); Department of Nano-Mechatronics, University of Science and Technology(UST)

Resume : Functional polymer membrane has been highlighted due to its higher functionality in separation processes for liquid and gaseous mixtures and in other important applications of membranes, such as bio-materials, catalysis production. In this study, sputtered Pt film was coated on PTFE membrane surface. The Ti film was inserted for improved adhesion between Pt film and PTFE membrane. Under negative electrical bias, the Pt film coated PTFE membrane showed almost 30% reduction of Cl- ions in NaCl solution. In addition, solution including nitrate ions was also investigated in this study. Selective ion transportation through Pt film coated PTFE membrane under electrical bias will be systemically presented using proposed mechanism and experimental results.

14:00

Hydride formation thermodynamics and hysteresis in individual Pd nanocrystals with different size and shape

X.PII.6

Authors : Svetlana Syrenova, Carl Wadell, Ferry A. A. Nugroho, Tina A. Gschneidtner, Yuri A. Diaz Fernandez, Giammarco Nalin, Dominika Świtlik, Fredrik Westerlund, Tomasz J. Antosiewicz, Vladimir P. Zhdanov, Kasper Moth-Poulsen, Christoph Langhammer
Affiliations : Department of Physics, Chalmers University of Technology, 412 96 Göteborg, Sweden Svetlana Syrenova; Carl Wadell; Ferry A. A. Nugroho; Tomasz J. Antosiewicz; Vladimir P. Zhdanov; Christoph Langhammer. Department of Chemistry and Chemical Engineering, Chalmers University of Technology, 412 96 Göteborg, Sweden Tina A. Gschneidtner; Yuri A. Diaz Fernandez; Giammarco Nalin; Kasper Moth-Poulsen Centre of New Technologies, University of Warsaw, Banacha 2c, 02-097 Warsaw, Poland Dominika Świtlik; Tomasz J. Antosiewicz. Department of Biology and Biological Engineering, Chalmers University of

Technology, 412 96 Göteborg, Sweden Fredrik Westerlund. Boreskov Institute of Catalysis, Russian Academy of Sciences, Novosibirsk 630090, Russia Vladimir P. Zhdanov.

Resume : Physicochemical properties of nanoparticles may depend on their size and shape and are traditionally assessed in ensemble-level experiments, which accordingly may be plagued by averaging effects. These effects can be eliminated in single-nanoparticle experiments. Using plasmonic nanospectroscopy, we present a comprehensive study of hydride formation thermodynamics in individual Pd nanocrystals of different size and shape, and find corresponding enthalpies and entropies to be nearly size- and shape-independent. The hysteresis observed is significantly wider than in bulk, with details depending on the specifics of individual nanoparticles. Generally, the absorption branch of the hysteresis loop is size-dependent in the sub-30 nm regime, whereas desorption is size- and shape-independent. The former is consistent with a coherent phase transition during hydride formation, influenced kinetically by the specifics of nucleation, whereas the latter implies that hydride decomposition either occurs incoherently or via different kinetic pathways. References: 1. Gschneidtner, T. A. et al. A Versatile Self-Assembly Strategy for the Synthesis of Shape-Selected Colloidal Noble Metal Nanoparticle Heterodimers. Langmuir 30, 3041-3050, (2014). 2. Syrenova, S. et al. Hydride formation thermodynamics and hysteresis in individual Pd nanocrystals with different size and shape. Nature Materials 14, 1236-1244, (2015).

14:00 Nanoforest of Hierarchical Core/Shell CuO@NiCo2O4 Nanowire Heterostructure Arrays on Nickel Foam for High-performance Supercapac **X.PII.7**

Authors : Chun Wu, Junjie Cai, Qiaobao Zhang, Ying Zhu, Kaili Zhang
Affiliations : Department of Mechanical and Biomedical Engineering, City University of Hong Kong, 83 Tat Chee Avenue, Hong Kong

Resume : Nickel foam supported CuO@NiCo2O4 nanoforests with mesoporous hierarchical core/shell structure are prepared by combining a facile, scalable, and cost-effective thermal oxidation method with a simple hydrothermal method followed by a calcination procedure. The smart hybridization of CuO nanowires and NiCo2O4 nanosheets into hierarchical core/shell array configuration results in remarkably enhanced electrochemical performances with high specific capacitance, excellent rate capability and good cycle performance compared with pure nickel foam supported NiCo2O4 nanosheets. A high specific capacitance of 1298.8 F g-1 at a current density of 1 A g-1 has been exhibited and excellent rate capability of about 96.3% capacitance retention at 5 A g-1 can be obtained. The CuO@NiCo2O4 based supercapacitor exhibits wonderful long cycle life with only 2.1 % capacitance loss after 2000 cycles and the coulombic efficiency maintains about 100% during the cycling. These excellent electrochemical performances demonstrate that the nickel foam supported hierarchical core/shell CuO@NiCo2O4 nanowire heterostructure array electrodes are highly desirable for application as advanced supercapacitor electrodes.

14:00 Supercapacitive behavior investigation of the activated microporous carbon derived from almond shell **X.PII.8**

Authors : Shaoran YANG, Chun WU, Kaili ZHANG
Affiliations : City University of Hong Kong, Tat Chee Avenue,

Kowloon, Hong Kong SAR.

Resume : The activated microporous carbon derived from almond shell has been successfully prepared through the activation process with KOH (C-2) and HNO3 (C-3). The activation results in microstructures with BET specific surface area of 1363.1 m2 g-1 with KOH treatment. And the content of Nitrogen reaches about 10 % with HNO3 activation. When evaluated as electrodes for supercapacitors, both of these two microporous carbon electrode materials exhibit high specific capacitance, good rate capability and excellent long cycle life. C-2 electrode possesses the specific capacitance as high as 286.1 F g-1 at 1 A g-1 and the retention of capacitance maintains at 84.1 % even at 1 A g-1. Furthermore, the Coulombic efficiency remains at 100% after 10000 cycles. These two methods to prepare the microporous carbon are facile and safety, and easy for mass production. Thus, it can provide a kind of readily available, renewable and cheap raw electrode materials for high performance EDLCs.

14:00 Sulfur Impregnated N, P-doped Hierarchical Porous Carbon as Cathode for High Performance Li-S Batteries **X.PII.9**

Authors : Junjie Cai, Kaili Zhang*
Affiliations : Department of Mechanical and Biomedical Engineering, City University of Hong Kong, 83 Tat Chee Avenue, Hong Kong

Resume : A two steps strategy has been exploited to prepare sulfur impregnated N, P-doped hierarchical porous carbon as cathode for high performance Li-S Batteries. A template-free method for the fabrication of N and P co-doped hierarchical porous carbon (HPC) were firstly used by simply pyrolysis of polyaniline aerogels synthesized in the presence of phytic acid. The resultant carbon show a high specific surface area and good electrical conductivity. For the application in Li-S batteries, sulfur impregnated N, P-doped hierarchical porous carbon hybrid material was produced by homogeneously mixing sulfur with N, P-doped HPC under heat treatment at 155℃. As cathode electrode, these sulfur impregnated N, P-doped HPC hybrid materials show high capacity and highly stable cycling performance, suggesting that the novel cathode have alluring prospect for Li-S batteries.

14:00 ORDERED β-CYCLODEXTRIN-FUNCTIONALIZED MCM-41: SYNTHESIS AND INVESTIGATION **X.PII.10**

Authors : Trofymchuk I.M., Belyakova L.A.
Affiliations : Chuiko Institute of Surface Chemistry, National Academy of Sciences of Ukraine, 17 General Naumov Str., Kyiv 03164, Ukraine

Resume : Ordered mesoporous MCM-41 silica is commonly used for the production of functionalized materials, such as adsorbents, catalysts, membranes, and sensors. In this research, we realized β-cyclodextrin(β-CD)-functionalized MCM-41 silica producing by postsynthesis grafting to hexagonally ordered aminopropyl-containing support. Aminopropyl-MCM-41 silica support was prepared by co-condensation of tetraethyl orthosilicate and (3-aminopropyl)triethoxysilane in the presence of cetyltrimethylammonium bromide. Surface grafting of β-CD onto aminopropyl-MCM-41 silica was carried out under mild conditions thought the activating agent (N,N'-carbonyldiimidazole) usage. Characterization of β-CD-MCM-41 silica was performed using XRD, TEM, chemical analysis, and low-temperature adsorption-desorption of nitrogen.

Hexagonally ordered pore structure of obtained silica was confirmed by XRD and TEM analyses, where the presence of diffraction peak at 2θ = 2.20 grad. is attributed to the (100) reticular planes, and the long-range array of tubular voids on the TEM images is observed. The estimated content of amino and β-CD groups on the surface of aminopropyl-MCM-41 and β-CD-MCM-41 silicas was 0.74 and 0.28 μmol/m2, respectively. So many unreacted amino groups may indicate that β-CD are mainly grafted at the entrance of the pores, preventing further penetration of oligosaccharide moieties to the inner pore surface with other anchoring sites. The pore size distribution plot (NLDFT model) confirms the complex pore structure of β-CD-MCM-41 silica with two types of mesopores (3.4 and 5.1 nm) as well as textural porosity within the sheet-like particles. β-CD-MCM-41 silica has high surface area (580 m2/g) and large pore volume (0.97 cm3/g).

14:00 A quantum chemical investigation of electronic and optical properties of fullerene linked acceptors dyads by conjugated bridges. **X.PII.11**

Authors : Massimo Ottonelli (a), Marina Alloisio (a), Ivana Moggio (b), Massimo Maccagno (a), Eduardo Arias (b)
Affiliations : (a) Dipartimento di Chimica e Chimica Industriale, Università di Genova, Via Dodecaneso 31, 16146 Genoa, Italy. (b) Centro de Investigación en Química Aplicada (CIQA), Blvd. EnriqueReyna 140, 25294, Saltillo, México.

Resume : Donor-acceptor molecules have received an increasing interest in fields such as: dye-sensitized solar cells, molecular electronics and non-linear optics thanks to their specific spectroscopic and electronic properties, which are related to the intramolecular charge transfer that occurs in these systems. In particular, fullerene derivatives are one of the most widely used electron acceptor unit because of their capacity to accept up to 6 electrons. On the other side, ferrocene, for its remarkable stability and strong electron donor ability, is supposed to be the most suitable counterpart to build an efficient donor-acceptor dyad, as reported in literature, where different fullerene/ferrocene hybrid systems with interesting properties have been proposed. In this work, we address a quantum chemical study on the structural, electronic and optical properties of novel push-pull macromole-cules based on fullerene-ferrocene groups linked by a phenyleneethynylene conjugated bridge, in order to better understand the structure-function relationship and the in-silico design of new donor-acceptor dyad materials for applications in the organic photovoltaic field.
Acknowledgement: We thank to Italian Ministry for Instruction University and Research (MIUR, PRIN project no. 2012a4z2ry) and Centro de Investigación en Química Aplicada (CIQA project no. 6236) for financial support.

14:00 High sensitive combustion gas sensors based on silicon carbide MOS structure **X.PII.12**

Authors : Jenica Neamtu 1, Florea Craciunoiu2, Dragos Ovezea1, Razvan Pascu 2
Affiliations : 1 National Institute for Research&Development in Electrical Engineering, 2 National Institute for Research&Development in Microtechnology, Bucharest Romania

Resume : Due to outstanding silicon carbide (SiC) properties, such as wide band gap, low dielectric constant, high breakdown voltage, good thermal conductivity, chemical stability in reactive environments, SiC sensors are capable of

operating properly at high temperatures and hostile environments. In this paper we present the palladium/silicon oxide/silicon carbide sandwich structures which are metal/oxide/semiconductor (MOS) devices. We investigate the temperature influence on the behaviour of hydrogen sensors based on MOSiC capacitors which use Pd as catalytic gates. The structures were fabricated on n-type 4H-SiC wafers, 0.015-0.028 ohm-cm resistivity, with two epitaxial layers: a buffer with a thickness of 0.5µm, and the active layer with a thickness of 7.9µm lightly doped. The silicon oxide layer, with different thicknesses, from 10 to 50 nm was thermally grown. A chip structure with three different areas: 200, 300, 400 µm has been developed in order to obtain a sensor array for hydrogen detection. The sensor response, measured on a Pd/SiO2/SiC structure, shows an important temperature dependence up to 200°C. After this threshold, the sensitivity remains practically constant. This behaviour can be associated with the presence of interface states, which affect sensor sensitivity at low temperatures. The gas sensing capability of Pd/SiO2/SiC sensors were tested at different H2 concentrations. The sensitivity of Pd/SiO2/SiC sensor is very good over 3 ppm H2: Ar.

14:00

Treatment of fly ash from power plant using thermal plasma

X.PII.13

Authors : Sulaiman AlMAYMAN 1, Imed Ghiloufi 2, Ibrahim AlShunaifi 1, Abdullah Albeladi 1, Meshal Aljuhni 1
Affiliations : 1 King Abdulaziz City for Science and Technology (KACST), National Center for Combustion & Plasma Technology, Riyahd, Saudi Arabia; 2 Al Imam Mohammad Ibn Saud Islamic University (IMSIU), College of Sciences, Riyadh, Saudi Arabia.

Resume : The objective of this work is to treat the fly ash produced from a power plant (PP). For this reason the PP was analyzed by many technics such as X-ray fluorescence (XRF), CHN Analyzer, Inductively coupled plasma (ICP), Nitrogen adsorption and desorption isotherms (BET). With these technics the composition, the chemical and physical proprieties of PP are determined. The treatment of PP is carried out into a plasma reactor with transferred arc plasma. To study the volatility of toxic element present in PP during the treatment of fly ash by plasma, a computer code was used. This model is based on the calculation of system composition using the free enthalpy minimization method, coupled with the equation of mass transfer at the reactional interface. The model enables the determination of the effects of various parameters (e.g., temperature, plasma current, and presence of oxygen in the carrier gas) on the toxic element volatility.

14:00

Protonic Conductivity of Dense BaZrO3 Ceramic Synthesized by Flash Pyrolysis Process for PCFC Applications

X.PII.14

Authors : Deepash Shekhar Saini, Debasis Bhattacharya
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Resume : Perovskite cubic BaZrO3 ceramic is prepared by the flash pyrolysis route. Rietveld refinement of XRD pattern of calcined powder at 900 °C, 1100 °C and sintered at 1600 °C describes that a single-phase compound is formed of an Pm-3m cubic crystal structure with a lattice constant a = 4.19352, 4.19370, and 4.19336 Å respectively. The HRTEM image of calcined powder at 1100 °C for 4 h shows nearly spherical in shape and is sub micrometer aggregates of nano-crystallites of 10–50 nm in size. The FESEM image of sintered pellet at 1600 °C for 8 h reveals highly dense nature

of BaZrO3. The observed Raman spectrum of BaZrO3 is assigned to have its source in the nanodomains with the symmetry different than cubic one. AC electrical properties reveal four relaxations. An equivalent circuit model with four RC loops in series is used to extract the electrical conductivity of BaZrO3 in 3% humidified O2. The total conductivity of BaZrO3 dense ceramic is found 7.3546 □ 10-5 S-cm-1 at 750 °C in 3% humidified O2. The giant dielectric constant (ε') of BaZrO3 is attributed to the Maxwell–Wagner polarization mechanism as well as to the thermally activated mechanism of charge carriers. The dielectric measurements were studied by fitting the electrical modulus with the Kohlrausch–Williams–Watts (KWW) function.

14:00 Effect of heat treatment on structural and optical properties of CdO films deposited by sol–gel method **X.PII.15**

Authors : I. Ben Miled*1, M.Jlassi 2, I.Sta 1, M.Hajji 3, and H. EZZAOUIA1.
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Resume : Abstract Transparent semiconducting thin films of cadmium oxide (CdO) thin films have been prepared by the sol-gel technique and was deposited by spin coating on slide glass substrates. And then the film has been annealed at 350, 400, 450, 500° C for 1 h. Effect of annealing temperature on the structural and optical properties of the film has been investigated. The XRD analysis reveals that the films are polycrystalline with (111) preferential orientation with cubic rock salt phase. The optical properties of the films were characterized by UV–Visible spectrophotometry. From optical analysis, it can be seen that there are an increases in the absorbance and decreases in the transmittance of the prepared films with the increasing of the annealing temperatures. The optical band gap value decreased with increasing the annealing temperatures. Keywords: Cadmium oxide, Thin films, sol gel, Structural and optical properties, annealing temperature.

14:00 Transferable Self-assembled monolayer modified crystalline ZnO as a hole transport layer for inverted organic solar cells **X.PII.16**

Authors : Cheng-Yu Chi, Chun-Han Shih, Sandeep Das, Hsiang-Ting Lien, Yian Tai*
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Resume : In general, zinc oxide (ZnO) is used as an electron transport layer in organic solar cells (OSC) owing to its high electron mobility, ease of fabrication, and most importantly, the suitable energy alignment. However, through this study, we present role of a self-assembled monolayer (SAM) modified ZnO thin film as an effective hole transport layer (HTL). Different SAMs modified ZnO were prepared, which later transferred onto the glass/ITO/ZnO/P3HT-PCBM substrate for use of them as HTL in inverted OSC architecture. SAMs modulate the work function of ZnO to make interfacial contact more ohmic, thus creates a direct

pathway of holes to the cathode. The fabricated device shows improved stability and comparable efficiency with respect to the OSCs utilizing MoOx as HTL.

14:00 High-performance ultraviolet photodetector design based on TiO2 thin film **X.PII.17**

Authors : K. Kacha1, F. Djeffal1,2,*, H. Ferhati1 and D. Arar1
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Resume : Recently, ultraviolet (UV) thin film photodetectors (PDs) have received much consideration in different field of research due to their applications environmental monitoring, optical communications and large-area displays. Optimization of photodetectors including new morphological aspects is indispensible to improve the thin film photodetector performance. In this context, this paper presents a numerical investigation including new interface grating morphology effects in order to optimize the photodetector performance and design parameters. In the present work, the impact of grating designs on the device behavior is studied using optical and electrical modeling and an optimized design is proposed to improve the UV absorbance of the photodetector. The specific photodetector studied is based on a Si/TiO2 structure, though qualitative findings are applicable to any thin film photodetector application. Si/TiO2 PD with optimized triangular grating exhibits an enhancement over conventional planar PDs. The purpose of this work is to find an optimal diffraction grating structure that would help in obtaining high optical and electrical performances.

14:00 P-type Li-doped Cu2O films for p-n heterojunction thin film piezoelectric nanogenerators **X.PII.18**

Authors : Kyung Su Cho, Do-Hee Kim, Han-Ki Kim
Affiliations : Department of Advanced Materials Engineering for Information and Electronics, Kyung Hee University, Yongin-si, Gyeonggi-do, 446-701, South Korea

Resume : We investigated characteristic of DC sputtered Li-doped Cu2O films to use as p-type layer for p-n heterojunction piezoelectric nanogenerators. The electrical, optical, morphological and structural properties of Li-doped Cu2O films were investigated as a function of Ar/O2 flow ratio during RF sputtering. In addition, microstructure and interfacial structure of the Li-doped Cu2O layer was analyzed by using a high resolution transmission electron microscope in detail. The p-type conductivity of the Li-doped Cu2O films was confirmed by Hall measurement. Furthermore, using the n-ZnO and p-Li:Cu2O layers, the p-n diode was fabricated and electrically characterized to confirm the p-type conductivity of Li:Cu2O layer. Obvious rectifying behavior can be observed in the p-n heterojunction diode, indicating the formation of p-type Li:Cu2O layer on n-ZnO. The semitransparent and flexible Li:Cu2O-ZnO heterojunction piezoelectric nanogenerators demonstrates the output power up to ~67.5 μW and piezoelectric potential screening effect in ZnO layer significantly reduced by existence of p-type Li:Cu2O layer. Based on performance of Li:Cu2O-ZnO heterojunction piezoelectric nanogenerators, we suggested a possible mechanism to explain the effect of p-type Li:Cu2O layer.

14:00 Polymer/nanostructured carbon composites with **X.PII.19**

stress dependent dielectric permittivity for electrostatic energy harvesters

Authors : J.Blums, K.Ozols, M.Knite
Affiliations : Institute of Technical Physics, Faculty of Material Science and Applied Chemistry, Riga Technical University, Riga, Latvia

Resume : The possibility to improve an efficiency of electrostatic harvesters by usage of polymer/nanostructured carbon (PNC) composites was investigated. In electrostatic harvesters the energy of mechanical oscillations is converted into electrical energy through deformation of dielectric layer between plates of charged capacitor. To increase the change of voltage during the deformation of dielectric layer between capacitor plates, its dielectric permittivity should decrease with tensile deformation. As a candidate for such a dielectric material PNC composite was chosen. Capacitor samples containing PNC dielectric layer were elaborated from 1) SVR-3L natural rubber with added curing ingredients (this is used as a matrix); 2) high structure Degussa™ Printex™ EX-2 carbon black with average particle size 30 nm (filler); 3) two brass electrodes (thickness of each electrode 2 mm). Thickness of the PNC composite layer for each sample is 1mm. The concentration of the filler in the composite layer was chosen to be from 2 up to 8 mass parts per 100 mass parts of rubber. Tensile and compressive deformation measurements conducted on PNC samples showed, that under tensile and compressive deformation dielectric permittivity of composite is changing non monotonically. The decrease of the dielectric permittivity with increasing of the tensile and stretching deformation of the dielectric layer was observed. It was also found, that character of dielectric permittivity change for both - tensile and compressive deformation - is different. The change of dielectric properties observed indicates about complex processes taking place in the PNC dielectric layer.

14:00

Ammonia gas sensing by microwave transduction : influence of hematite nanorods aspect ratio

X.PII.20

Authors : Guillaume Bailly, Jérôme Rossignol, Valentin Collin, Brice de Fonseca, Pierre Pribetich, Didier Stuerga
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Resume : Hematite α-Fe2O3 spindle-like particles with controlled aspect ratio were prepared via an environment-friendly and low cost microwave route, without any organic additive. Scanning electron microscopy (SEM) and transmission electron microscopy (TEM) analysis were conducted to characterize the structure and the morphology of synthesized particles. Possible oriented-attachment-based formation mechanisms of the particles were discussed. Gas sensing experiments for the detection of ammonia concentrations with hematite sensitive layers were conducted using an original microwave transduction. Its main advantages are the possibility to carry room-temperature measurements even with electrical insulator, and the acquisition of data over a wide range of frequencies. The sensor microwave design involves a conductor-backed coplanar waveguide (CBCPW) on which the hematite sensitive layer is deposited. Hematite deposition was realized via a simple doctor-blade protocol on the most responsive areas, identified by Near-Field Microwave Microscopy (NFMM). A comparative microwave gas sensing study was conducted to evaluate the gas response of these morphologies upon ammonia exposure at room temperature, and revealed that each morphology presents a significantly

different behavior upon gas adsorption. This work is part of a general study on the relation between morphology and properties in the hematite case.

14:00 Body-attachable active matrix temperature sensor array of polyaniline nanofibers **X.PII.21**

Authors : Soo Yeong Hong1, Yong Hui Lee1, Heun Park1, Sang Woo Jin2, Yu Ra Jeong1, Junyeong Yun1, Jeong Sook Ha1,2
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Resume : Recently, there has been remarkable accomplishment in the field of stretchable electronics including display panels, radio frequency electronics, light emitting diodes (LEDs), acoustic devices, strain, and pressure sensors. Stretchable devices are required to ensure that no performance deterioration occurs due to body movements when electronics are applied to non-coplanar surfaces such as the human body. In this study, we report on the fabrication of a stretchable polyaniline nanofiber temperature sensor array with an active matrix (AM) consisting of the SWCNT thin film transistors (TFTs). In order to achieve mechanical stability under an externally applied strain, a specially designed soft Ecoflex substrate is used with locally implanted SWCNT TFTs and temperature sensors on stiff poly(ethylene terephthalate) films. Thus, the SWCNT TFTs are protected from the applied strain, and they are electrically connected via embedded interconnections of liquid metal Galinstan. Owing to the embedded Galinstan interconnections, SWCNT TFTs, LED arrays, and temperature sensors maintain their performance under the deformations such as bending and stretching. In addition, the fabricated 5 × 5 AM temperature sensor array can be easily attached to the skin owing to its thin film structure and use of the soft and sticky Ecoflex. The temperature sensor exhibits a high resistance sensitivity of 1.0 %/°C and a response time of 1.8 s in the temperature range from 15 to 45 °C. The integrated temperature sensor array with the SWCNT TFT-based AM backplane on the stretchable substrate gives mechanical stability under biaxial stretching of 30%, and the resultant spatial temperature mapping does not show any mechanical or electrical degradation. This work clearly suggests the high potential application of our stretchable AM temperature sensor array to realize high performance skin attachable electronic skin devices.

14:00 LTCC packaging for lab-on-CMOS applied in cell health status monitoring **X.PII.22**

Authors : Joni Kilpijärvi (1), Maciej Sobocinski (1), Niina Halonen (1), Antti Hassinen (2), Bathiya Senevirathna (3), Someshekar B. Prakash (3,4), Peter Möller (5), Pamela Abshire (3), Elisabeth Smela(6), Sakari Kellokumpu (2), Anita Lloyd Spetz (5)
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Resume : Pollution exposure of people living in urban areas is a health risk as the concentration of toxic compounds and particles is high in these areas. It is known that small particles go through the airways to the lungs and eventually enter the blood circulation. Nowadays nanomaterials are also used more extensively. Therefore, easy to use devices for biosafety evaluation of these materials are very interesting. Cell viability monitoring is one way to characterize biosafety of materials including nanoparticles. Traditionally, this is performed with stain based cytotoxicity evaluation kits. These measurements are expensive, laborious and provides only end-point measurements. Best way to tackle these problems is Lab-on-a-chip (LOC) concept, which integrates various laboratory functions on a miniaturized device. In this work a LOC device with cell viability measuring CMOS chip based on capacitance sensing was built. Healthy cells attach and spread out on the surface of the chip, while dying cells ball-up and this change in capacitance can be measured. The challenge is related to the packaging of this sensor chip. In this work, low temperature co-fired ceramic (LTCC) technology was combined with flip-chip bonding using different epoxy adhesives. Chip packaged in LTCC module was then integrated with printed circuit board, data acquisition and measurement-controlling software. Reliability, biocompatibility and cell viability measurements were successfully performed and will be reported.

14:00 Polymer based piezoelectric sensing system built by aerosoljet printing **X.PII.23**

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Resume : People having diabetes (according to WHO these were 9 % of the adult world population in 2014) often suffer from foot ulcers caused by reduced blood flow and nerve damage. For those people it is extremely important to wear well-fitting shoes to avoid additional stress to their feet, and successive ulcers and amputation. The piezoelectric sensor presented here could be worn constantly and help to monitor changes in the patients feet and to adapt their footwear. We have produced a flexible piezoelectric sensor, completely based on polymers. The piezoactive material is poly[(vinylidenefluoride-co-trifluoroethylene] [P(VDF-TrFE)]. The electrodes and the conductive paths are made of PEDOT:PSS with the co-solvent DMSO. The sensor has been built up by maskless aerosoljet printing on an adhesive polyester foil substrate. This process allows the printing of very fine structures in the µm-range, enabling high lateral resolution. The sensor produced for demonstration has a surface area of 0.25 mm2 and a total thickness of ~170 µm. Taking processes and materials together, we obtain a flexible and robust piezo system that can be applied on a high variety of surface materials and shapes (including arbitrarily

shaped 3D surfaces and textiles). These characteristics suggest the potential use of the system in medical applications as for example in specially designed footwear for diabetes patients.

14:00 LiNi1/3Co1/3Mn1/3O2 based suspensions as catholyte for semi solid flow batteries **X.PII.24**

Authors : Jordi Jacas Biendicho,*[a] Cristina Flox,[a] Laura Sanz,[a] and Joan Ramon Morante,[a,b]
Affiliations : [a] Catalonia Institute for Energy Research, Jardins de les dones de Negre 1, 08930 Sant Adrià del Besos, Barcelona, Spain. [b] Department d'Electronica, Facultat de Física, Universitat de Barcelona, Martí i Franques 1, 08028 Barcelona, Spain.

Resume : Semi Solid Flow Batteries (SSFB) are batteries in which both positive and negative suspensions, catholyte and anolyte, respectively, are pumped from reservoir tanks to electrochemical cell to release energy. SSFB preserve typical advantages of Redox Flow Batteries (RFB); flexibility in configuration and operation as well as energy and power decoupling, while the use of alkaline redox-active materials and organic solvents maximizes energy density of the system e.g. 309 Whkg-1[1]. LiNi1/3Co1/3Mn1/3O2 (LNCM) based suspensions as catholyte for SSFB have been prepared by magnetic stirring and characterized by galvanostatic charge/discharge and electrochemical impedance spectroscopy (EIS). The resistance and electrochemical performance of cells (vs. Li/Li+) are affected by the content of superconductive Ketjen Black (KB) in suspensions. In static conditions, a cell with 11.87 and 13.97 % in volume of KB and LNCM based suspension, respectively, delivers high capacity 130 mAhg-1 at 5 mAcm-2 and a coulombic efficiency of 90 % over 10 injections. Impedance analysis show that the high frequency semicircle in Z' vs Z'' plots is attributed to a contact resistance and fitted using a parallel combination of a resistor with a Constant Phase element (CPE). In flow conditions, cell potential depends on applied current as well as operation time. The last has been characterized by EIS and discussed in terms of suspension stability over time. [1] Q. Huang and Q. Wang, ChemPlusChem, 2015, 80 (2), 312-322.

14:00 Epitaxial NiO/ZnO nanowire-heterostructures by vapor phase growth **X.PII.25**

Authors : Navpreet Kaur*1, Elisabetta Comini1, Dario Zappa1, Nicola Poli1, Matteo Ferroni1, Roberta Ciprian1, Angela Bertuna1, Marco Campanini2 and Giorgio Sberveglieri1
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Resume : One-dimensional (1D) nanostructures, in particular, semiconducting metal-oxide nanowires have captured considerable attention owing to their remarkable performance as gas sensors, biosensors, solar cells, etc. [1]. ZnO (n-type) features a 3.37 eV band gap, non-toxic,environmentally stable, and, most abundant elements in earth's crust. Moreover, NiO (p-type) possess wide bandgap (3.6–4.0 eV) and is used for electro- chromic devices. In literature these two semiconducting materials has been widely investigated. Further, in nanomaterials based hetrostructures, due to strong heterointeractions between the closely packed interface, their performance is considered as more superior and complex. Herein, we report on the novel preparation and characterization of epitaxial NiO/ZnO

heterostructures, consisting of inner NiO NWs [2] and outer ZnO NWs obtained through vapor-phase method. The surface morphology of the nanowires was investigated by using scanning electron microscopy (SEM) while, for structural characterization GI-XRD, the transmission electron microscopy (TEM), and Raman spectroscopy were performed. The diameter of NiO NWs and NiO/ZnO heterostructure was found to be 16-50nm and 80-90nm respectively. The GI-XRD spectra shows that these nanowires have crystalline structures. Further, the TEM study confirms the epitaxial growth of ZnO nanowires on the NiO nanowires. These hetrostructures have potential to be used for gas sensing applications. References: [1] E. Comini et al. 179 (2013) 3. [2] N.kaur et al.120 (2015) 760.

14:00 GROWTH AND PROPERTIES OF Zn1-xFexO THIN FILMS DEPOSITED BY SPRAY PYROLYSIS. **X.PII.26**

Authors : E.M.ELJALD et al
Affiliations : university mohammed V, faculty of science laboratory physics of materials

Resume : Various Zn1-xFexO (x = 0, 3, 5, 7, 10, 15 and 20 at%) thin films were deposited on glass substrate at 450°C by the spray pyrolysis technique. This paper describes the effect of doping on the composition, structural, surface morphology, optical and electrical properties. The structural properties and the morphology of the films were investigated by X-ray diffraction (XRD), Scanning Electron Microscopy (SEM) and Atomic Force Microscopy (AFM). The XRD and SEM analyses indicate that the films are polycrystalline and textured with c axis of the wurtzite structure along the growth direction. The results show that the surfaces are homogeneous and the chemical composition close to the nominal one as confirmed by energy dispersive analysis of X-rays (EDAX). The AFM spectra reveal that the surfaces have a large roughness. The optical properties were studied using an UV-Visible-NIR spectrophotometer. The films are highly transparent and weakly absorbent in the visible region. The effect of iron doping on the photoluminescence of the films was also studied. The lowest resistivity of 2.25 10-3 □.cm was obtained for the sample Zn0.97Fe0.03O.

14:00 Study of TiO2 nanotube arrays by simultaneous grazing incidence small and wide angle X-ray scattering **X.PII.27**

Authors : Krunoslav Juraic (1), Milivoj Plodinec (1), Irena Kerekovic (1), Davor Gracin (1), Andreja Gajovic (1), Sigrid Bernstorff (2)
Affiliations : (1) Rudjer Boskovic Institute, Bijenicka cesta 54, 10000 Zagreb, Croatia; (2) Elettra-Sincrotrone Trieste, SS 14, km 163.5, 34149 Trieste, Italy

Resume : TiO2 is one of the most intensively investigated compounds in material science due to its essential properties. It is a wide band gap semiconductor having band-edge positions appropriate for solar cell applications and for hydrogen generation by water splitting. It is also known as a non-toxic, environment friendly, corrosion-resistant material. Nano-forms of TiO2 such as nanoparticles, nanorods, nanowires and, in particular nanotubes can be used as photo-electrode in dye sensitized solar cells. Conversion efficiency of solar cells can be significantly improved by using oriented nanorod-like materials on top of transparent conductive oxide. For this purpose we prepared TiO2 nanotube arrays by anodizing titanium thin film deposited on

ZnO covered glass substrate. Initial Ti films were prepared by evaporation or magnetron sputtering. Diameter and length of nanotubes were controlled by parameters of anodizatio mainly voltage and etching time. The structural properties of obtained TiO2 nanotubes arrays were estimated upon simultaneous small and wide angle x-ray scattering under grazing incidence geometry. Results will be also correlated by deposition parameters and results obtained by high resolution electron microscopy, scanning electron microsopy and Raman spectroscopy. It will be also discussed possible application in photovoltaic devices.

14:00 Dioxaborine Cyanine Dye as a Photoluminescence Probe for Sensing of Carbon Nanotubes **X.PII.28**

Authors : M. AlAraimi1,4,*, P. Lutsyk1,2, M. Shandura3, Yu. Piryatinski2, A. Verbitsky2 and A. Rozhin1,*
Affiliations : 1. Nanotechnology Research Group, Aston Institute of Photonic Technologies, School of Engineering & Applied Science, Aston University, Aston Triangle, B4 7ET Birmingham, UK. 2. Institute of Physics, National Academy of Sciences of Ukraine, 46, prospekt Nauky, 03680 Kyiv, Ukraine. 3. Institute of Organic Chemistry, National Academy of Sciences of Ukraine, 5 Murmanska str., 02660 Kyiv, Ukraine. 4. Engineering Department, Al Musanna College of Technology, Muladdah Musanna, Sultanate of Oman.

Resume : Carbon nanotubes (CNTs) exhibit unique physical and chemical properties that are different from other materials due to their extreme aspect offering a number of exciting applications as reinforced plastics, conductive composites, sensors and photonic devices[1]. The CNTs production facilities across the globe have reached of thousands of metric tons. However, concerns have been raised, with most studies agreeing, that CNTs pose a significant potential threat to health and environment. Therefore, development of efficient sensing techniques is needed for their detection. Previously, our group reported on CNTs sensing using newly synthesized Dioxaborne (DOB) dyes [2] and well known cyanine dyes [3]. DOB dye showed promising results towards CNT sensing. The neat dye has monomeric and dimeric forms in water and while interacting with CNT photoluminescence (PL) of the dye is quenched, PL of CNT is red shifted and new PL peaks in the near infra-red range of CNT emission appeared. Present work demonstrates dramatic changes in the properties of DOB with time and its consequence on the mixture of single wall CNTs (CoMoCat, South West NanoTechnologies) and the dye using absorption and PL spectroscopy. The properties of neat DOB dye change with time resulting in reduction of the monomeric and dimeric peaks. The monomeric peak of DOB solution dramatically decreases with few days and a new peak appears due to either aggregation or degradation state of monomeric molecules. The intensity of latter is 80% higher than the former. In the mixture of the dye and CNT, quenching of PL peaks was observed overnight for (6,5) and (7,5) CNT chiralities, whereas PL intensity for the (8,4) chirality was practically unchanged. Thus, we evidence a high selectivity of the dye interaction towards CNT chirality opening up a new way for selective sensing of CNTs.
Acknowledgements: The work was supported by NATO SPS project (NUKR.SFPP 984189) and EU FP ‘Horizon-2020’ Marie Skłodowska-Curie Individual Fellowship (FOC4SIP, 654733). References: [1] M. F. L. De Volder Science, 339 , pp. 535-539. (2013) [2] M. Shandura, et al., Sensor Letters, vol. 12, pp. 1361-1367, 2014. [3] P. Lutsyk, et al., " Light: Science & Applications, 5, e16028 2016.

14:00 Theoretical study of the carrier effective mass in diluted III-N-V semiconductor alloys using 10-band k.p model **X.PII.29**

Authors : K. Chakir, C. Bilel, M.M. Habchi, A. Rebey, and B. El Jani
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Resume : The dependence of carrier effective mass of GaNxAs1-x, InNxP1-x, InNxAs1-x, and InNxSb1-x alloys on nitrogen content is theoretically investigated using a 10-band k.p model. The electron effective mass m*e at the bottom of conduction band in GaNxAs1-x and InNxP1-x exhibits a gradual increase as a function of N concentration in the range 0-1% and a decrease for x between 1 and 5 %. However, the behavior of m*e in InNxAs1-x and InNxSb1-x shows a strongly decrease in all studied x-range. Our theoretical results are compared with the available data reported in the literature. On the other hand, contrary to heavy-hole effective mass m*hh, the light-hole effective mass m*lh in all studied alloys is significantly affected by nitrogen states which modify the non-parabolicity of the LH band. The modification of the carrier effective mass affects the transport and mobility properties of the III-N-V alloys. Keywords: Diluted III-N-V alloys; 10-band k.p model; carrier effective mass. * Corresponding author: ahmed.rebey@fsm.rnu.tn

14:00 New magnetosensitive nanocomposite materials for acoustoelectronic sensors **X.PII.30**

Authors : Kuznetsova I.E.1, Kolesov V.V.1, Kashin V.V.1, Anisimkin V.I.1, Zaitsev B.D.3, Shikhabudinov A.M.3, Gorshenev V.N.2, Verona E.1
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Resume : The control the magnitude of magnetic fields generated by different technical devices is an important ecological problem. In the paper for development of magnetic sensors the using acoustoelectronic technology is proposed. In this case the sensor will consists of the acoustic delay line with magnetosensitive film deposited on its surface between interdigital transducers. The variations of magnetic field will lead to changes of magnetic film properties that will cause the changes of acoustic wave parameters. The analysis showed that it is possible to use the thin layers of photoresist (Shipley S1805) with embedded nanoparticles of carbonyl iron as magnetosensitive film. As piezoelectric waveguides were used lithium niobate and quarts plates. The thickness of nanocomposite film produced by using spin coating method was not more 5 micron. The presence of the film does not lead to the significant attenuation of the acoustic waves propagating in delay line. The analysis of the influence of softener (n-methil-pyratidone) which was added into the photoresist on magnetosensitivity of developed films have been carried out. The element analysis, IR spectroscopy, X-ray analysis, XPS-spectroscopy, AFM microscopy of the developed materials have been also carried out. The work is supported by grant Russian Science Foundation #15-19-20046.

14:00 Optimization in p-doped GaNAsBi/GaAs SQWs **X.PII.31**

operating at 1.55µm.

Authors : I. Guizani, K. Chakir, C. Bilel, M.M. Habchi, A. Rebey*, B. El Jani
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Resume : We have theoretically studied optical properties of p-doped GaNAsBi/GaAs Single Quantum Well in order to reach the 1.55µm telecommunication wavelength. The calculation are carried out by solving selfconsistently the band (16×16) Kane Hamiltonien combined with the Poisson equation for the hole charge density. We have investigated the effect of p doping density in the well on the subband energies, potential Fermi level and the confining hole density distribution for specific couple (well width Lw,Bi composition y), with respect of confinement conditions. The increase of doping density blueshifts the fundamental transition. Furthermore, the case of doped barrier has been discussed. Based on these results, potential applications in long wavelength range are proposed.

14:00 A hybrid model for the design and optimisation of flexible vanadium dioxide nanoparticle thermochromic films **X.PII.32**

Authors : Christian Sol, Mark Portnoi, Alaric Taylor, Radhika Poduval, Ivan Parkin, Ioannis Papakonstantinou
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Resume : As cities grow and become more densely populated, there is a increasing issue of heat management, with buildings expending significant energy resources to maintain comfortable living temperatures. In many parts of the world, this entails the use of both heating and cooling during daylight hours depending on ambient temperatures. Due to the variation in the desired temperature modulation classical solutions can become counter productive in their aim of maintaining comfortable temperatures. To avoid such counter productivity, it is important to employ adaptive intelligent solutions which are able to switch their functionality based on circumstance. Here, we present a model for the design and optimisation of thermochromic smart windows based on the switching properties of vanadium dioxide (VO2) nanoparticles. In recent years vanadium dioxide has generated a broad range of interest due to its heat-mediated transition between a monoclinic distorted-rutile phase and a tetragonal rutile phase, which occurs at a critical temperature tunable via doping with tungsten. The phase transition of vanadium dioxide significantly modulates its optical properties, with the high temperature tetragonal state absorbing considerably more infrared radiation than the lower temperature monoclinic state due to a reduction in band-gap energy. It is such that a window coated with a composite polymer-nanoparticle film may passively vary its transmission of heat based on the ambient temperature, in doing so reducing the variation in temperature from the critical temperature and thus reducing energy usage in temperature management. In comparison to vapour deposited VO2 thin films, VO2 polymer-nanoparticle films may be retrofitted to existing windows and have reduced processing costs. We quantify the smart window performance over the transition between hot and cold state with the two key metrics of this field, transmission modulation of solar irradiance ΔTsol and transmission modulation of solar luminosity ΔTlum; an ideal window design will maximise ΔTsol whilst minimising ΔTlum. The model presented combines both finite-difference-time-domain (FDTD) and Monte Carlo

ray-tracing to create a hybrid model capable of modelling both micro- and macroscopic properties of a material composite. Specifically, FDTD can be used to model the optical response of nanoparticles of any geometry not otherwise available with analytical techniques, enabling the design and optimisation of novel nanoparticle geometries with improved modulation of infrared radiation. The results from our FDTD studies are then used in our C++ coded ray-tracer to generate probabilities for absorption, scattering and differential scattering during the transmission of single photons through the window; this process is then repeated many times to build up a macroscopic understanding of the properties of the window. Uniquely, the use of our hybrid model enables us to model both specular and diffuse transmission, from which we can investigate the level of haze resulting from the nanoparticles, a property that is often overlooked but very important in nano-particulate window design.

14:00 Hybrid Plasmon-Graphene System for Determination of Adenine **X.PII.33**

Authors : Christa Genslein (1), Peter Hausler (2), Eva-Maria Kirchner (1), Alessa Rolka (1), Antje J. Baeumner (1) ,Thomas Hirsch (1),
Affiliations : (1) Institute of Analytical Chemistry, Chemo and Biosensors, University of Regensburg, Regensburg, Germany (2) Sensor Application Center, OTH Regensburg, Regensburg, Germany

Resume : A receptor surface based on a hybrid gold nanohole array combined with graphene was prepared and used to detect adenine by Surface Plasmon Resonance (SPR) technique. Surface plasmon resonance depends on the dielectric medium at the vicinity and makes it a quasi-universal detector to a variety of analytes. The label-free nature enables a fast, specific, and sensitive analysis of molecular interactions. However, detection of highly diluted concentrations and small molecules is still challenging. Hybrid plasmon-graphene systems can improve the performance of standard SPR devices. Graphene, a 2-D lattice of sp2-hybridized carbon atoms arranged in a honeycomb structure is an attractive receptor as it omits any bulk phase and therefore allows fast response times. The interplay of the plasmonics of metal nanostructures with graphene photonics modulates and enhances locally the electromagnetic field. Amplification arises from localized surface plasmons at the nanostructures and lead to an increasing capability for sensing. The nanohole arrays, fabricated by nanosphere lithography show enhanced SPR sensitivity in changes of refractive index in close proximity to the surface compared to a film of continuous gold. A deposition of chemically derived graphene oxide enables the binding of planar molecules with aromatic systems via π-stacking. The binding of the model analyte adenine verified the enhanced sensitivity by achieving approximately three times lower limits of detection.

14:00 Trap state passivation induced efficiency enhancement in ZnO based inverted BHJ solar cells using C70 bridge **X.PII.34**

Authors : S. Kumar, D. Panigrahi, and A. Dhar
Affiliations : Department of Physics, IIT Kharagpur, Kharagpur-721302, India

Resume : The interface quality of ZnO and the photoactive polymer blend is of utmost importance in the performance of organic-inorganic hybrid photovoltaic devices. The chemically prepared ZnO electron transporting layer often

produces a surface unacceptable for efficient electron extraction and leads to degrade the photovoltaic performance. Herein, we propose a simple technique to enhance the charge collection efficiency of ZnO cathode electrode by thermally evaporated C70 between the ZnO and the photoactive PCDTBT: PC71BM polymer blend. Our investigations show that C70 interlayer efficiently bridges the gaps between ZnO and the polymer blend reducing accumulation of the charges at the interface and thus minimizing the recombination probability. It also plays crucial role in passivating ZnO electrode against traps due to adsorbed chemical species. The inclusion of C70 interlayer into our devices led to a substantial increase in device performance with PCE reaching close to 4%, an increment by a factor of 2 compared to our control devices.

14:00 Magnetic and Spectroscopic investigations of Ag, Au and Cr doped CeFe2 compounds **X.PII.35**

Authors : Rakesh Das1, Mukul Gupta2, and S.K. Srivastava1
Affiliations : 1 Department of Physics, Indian Institute of Technology Kharagpur – 721302, W. B., India 2 UGC-DAE Consortium for Scientific Research, University Campus, Khandwa Road, Indore 452 001, India

Resume : In rare-earth (R) - transition metal (TM) intermetallic compounds, the conduction electrons present in the TM experience a local exchange interaction with the R f electrons through a long range RKKY type coupling. This mechanism often leads to the occurrence of complex magnetic phases. The Laves phase compound CeFe2 is an unusual member of the RFe2 family - it has a relatively low Curie temperature (TC ≈ 230 K), an anomalously low lattice constant (7.3 Å), and a reduced magnetic moment (≈ 2.3 μB/f.u.) compared to others, and is on the verge of a magnetic instability [1]. A small but suitable change in electronic structure, caused by doping with certain 3d, 4d, 5d elements or by applying pressure, causes an additional ferromagnetic (FM) to antiferromagnetic (AFM) phase transition at low temperature [2]. In the present work, we investigate the effect of substitutional impurities Cr, Ag and Au in CeFe2. The X-ray Photoelectron Spectroscopy (XPS) measurements establish the mixed valence of Ce in CeFe2 and in the alloys of all compositions. Magnetization measurements on samples with all the impurities and concentrations confirm the presence of a paramagnetic (PM) to ferromagnetic (FM) phase transition at ~ 230 K. Further, the Ag and Au substituted samples are found to retain their FM phase down to 5 K. For Cr impurities, however, there appears a second, possibly FM to antiferromagnetic (AFM), phase transition at a concentration-dependent temperature below 50 K. Strain induced jumps in the magnetization curves and the asymmetric nature of the hysteresis curves are indicative of the FM to AFM phase transition. The Arrott plots for the Cr impurities suggest the second transition to be of the first order. X-ray Absorption Spectroscopy (XAS) is used to investigate d - f hybridizations in these compounds. The hybridization, as determined from the f 0/f 1 peak area ratio, is found to be dependent on Cr concentration and follows the concentration dependence of PM to FM transition temperature. Further, the magnetization results for the Cr doped samples reveal a martensitic nature, which is rarely found in this class of pseudobinary compounds, rendering these to be potential candidates for multifunctional applications. References 1. S. B. Roy and B. R. Coles, J. Phys. F: Met. Phys. 17 (1987) L215. 2. A. Haldar, K. G. Suresh, A. K. Nigam, Phys. Rev. B 78 (2008) 144429.

14:00 Numerical simulations of natural convection in an asymmetrically heated vertical channel with an adiabatic auxiliary plate

X.PII.36

Authors : S. Taieb 1, *, A. Babeer2, H. Laatar 3
Affiliations : 1 LETTM, Département de Physique, Faculté des Sciences de Tunis, Tunis El Manar University, 1060 Tunis, Tunisia 2Physics Department, Faculty of Sciences,Jazen University, Jazen Saudi Arabia 3 Département de Physique, Faculté des Sciences de Bizerte, University of Carthage, 7021 Jarzouna, Tunisia

Resume : This communication examines the numerical simulation of air natural convection in a vertical channel with an auxiliary plate. The channel is asymmetrically heated with a uniform heat flux, while the auxiliary plate is adiabatic. The computational procedure is made by solving the unsteady two dimensional Navier-Stokes and energy equations. This nonlinear system is integrated by a finite volume approach and then solved in time using the projection method, allowing the decoupling pressure from velocity. An adiabatic auxiliary plate is placed at different vertical positions along the centerline and at different lateral locations. The aim of this work is to conduct a detailed numerical study to analyze the effects of the auxiliary plate position on the natural convection behavior in the vertical channel for four values of the modified Rayleigh numbers Ram=102, Ram=103, Ram=104 and Ram=105 (steady regime). The numerical results (velocity, pressure and temperature fields) give detailed information about the evolution of the flow structure. In addition, they permit the computing of the quantities of engineering interest, such as the Nusselt number, the induced mass flow rate and the pressure at the mid-plane. The off-center positioning was found to be the best in terms of mass flow rate and heat transfer enhancement. The change in the auxiliary plate position has a minor effect on the Nusselt number with a variation not exceeding ±5%. The effect on the mass flow rate is more explicit. Indeed, there is a particular position which slightly improves it, while the remaining positions cause more or less significant reductions that can reach 50%. The auxiliary plate could be a simple and cheap tool that can be integrated in natural ventilation systems to control the mass flow rate.

14:00 Electrophoretic Deposition of Nanoparticles for Low Temperature Photo-thermal Solar Receptors

X.PII.37

Authors : SHEHAYEB Sanaa (1,2), DESCHANELS Xavier (1), KARAME Iyad (2), GHANNAM Leila (2), TOQUER Guillaume(1)
Affiliations : (1)Laboratoire de Nanomatériaux pour l'Energie et le Recyclage Institut de Chimie Séparative de Marcoule UMR 5257 - Bât 426 - CEA Marcoule BP 17171 - 30207 Bagnols sur Cèze, France (2) Laboratoire de Catalyse Organometallique et Chimie de Coordination, LCOCC Hadath-Liban

Resume : To limit the consumption of fossil fuels, hot water production by using photothermal solar receptors is growing in importance. An efficient photothermal receptor have to display a high solar absorptance ($\alpha>0.9$), in the UV-VIS and near-IR regions (0.5-2µm) with a low thermal emittance ($\varepsilon<0.1$), in the mid-far infrared region (2-20µm) [1-3]. Here we report for the first time the formation of the solar selective CuO layer by the electrophoretic deposition (EPD) of CuO nanoparticles. A tandem absorber-reflector system is formed of CuO thin film and a highly IR reflecting metallic substrate, respectively. CuO suspensions are characterized by Dynamic light scattering (DLS) and Small angle X-Ray diffraction (SAXS) where they show to be stable during the time of the experiment. X-ray diffraction (XRD), scanning electron microscopy (SEM), UV-vis-NIR spectra and Fourier

transform (FTIR) spectra are used to characterize the composition, microstructure and the final optical properties of the films obtained. These CuO tandem systems obtained by EPD exhibits the required optical properties in comparison to traditional processing techniques usually used. [1] Bogaerts WF, Lampert CM. Materials for Photothermal Energy Conversion. Journal of Materials Science. 1983;18:2847-75. [2] Charlot A, Bruguier O, Toquer G, Grandjean A, Deschanels X. Nanocomposites derived from silica and carbon for low temperature photothermal conversion. Thin Solid Films. 2014;553:157-60. [3] Charlot A, Deschanels X, Toquer G. Submicron coating of SiO2 nanoparticles from electrophoretic deposition. Thin Solid Films. 2014;553:148-52.

14:00 One dimensional core@shell nanostructures by plasma assisted vacuum deposition **X.PII.38**

Authors : A. Nicolas Filippin, Manuel Macias-Montero, Juan R. Sanchez-Valencia, Zineb Sagui, Paul A. Midgley, Pierre Burdet, Jesús Idígoras, Juan A. Anta, Angel Barranco, Ana Borras
Affiliations : Nanotechnology on Surfaces Laboratory, ICMS Materials Science Institute of Seville (CSIC-US). C/ Americo Vespucio 49, 41092, Seville (Spain); Department of Materials Science and Metallurgy, University of Cambridge, 27 Charles Babbage Road, CB3 0FS, Cambridge (United Kingdom); Departamento de Sistemas Físicos, Químicos y Naturales Universidad Pablo de Olavide, Carretera de Utrera km1, 41013 Seville (Spain)

Resume : Heterostructuration of one dimensional nanomaterials provides a straightforward route for the fabrication of multi-functional nanostructures which is the first step in the realization of single-wire devices. The idea behind is to fabricate 1D nanostructures completely capable of working as a whole devices by themselves, without the necessity of extra components to meet a certain application or set of applications. This approach has already been implemented in many fields such as electrochemistry, chemical sensing and energy generation. We have developed during the last years a reliable full vacuum / plasma methodology for the fabrication of supported core@shell nanowires and @multi-shell nanotubes with controlled shells composition, microstructure and porosity [1-5]. Several examples will be shown for the fabrication of semiconducting organic and inorganic nanotubes and core@shell/multishell nanowires and metal decoration of 1D nanostructures on processable substrates with advanced performances as photoelectrodes in solar cells, nanogenerators and nanosensors. [1] Alcaire, M. Soft plasma processing of organic nanowires: a route for the fabrication of 1D organic heterostructures and the template synthesis of inorganic 1D nanostructures. Nanoscale 2011, 3, 4554-4559. [2] Macias-Montero, M. Vertically Aligned Hybrid Core/Shell Semiconductor Nanowires for Photonics Applications. Adv. Funct. Mater. 2013, 23, 5981–5989. [3] Macias-Montero, M. Laser Treatment of Ag@ZnO Nanorods as Long-Life-Span SERS Surfaces. ACS Appl. Mater. Inter. 2015, 7, 2331–2339. [4] Alcaire-Martin, M. Highly Porous ZnO Thin Films and 1D Nanostructures by Remote Plasma Processing of Zn-Phthalocyanine. Plasma Proc. Polym. 2015 10.1002/ppap.201500133 [5] Filippin, A. N. Vacuum template synthesis of multifunctional nanotubes with tailored nanostructured walls. Scientific Reports 2016 (just accepted)

14:00 Comparison of Conventional vs. Liquid Injection **X.PII.39**

MOCVD of BaMgF4 thin films

Authors : Sergio Battiato,a, Jean-Luc Deschanvres,b, Hervé Roussel,b, Laetitia Raepenne,b, Béatrice Doisneau,b, Guglielmo G. Condorelli,a, David Muñoz-Rojas,b, Carmen Jimenez,b*, Graziella Malandrino,a*
Affiliations : a Dipartimento di Scienze Chimiche, Università degli Studi di Catania, INSTM UdR-Catania, Catania, 95125, Italy; b Laboratoire des Matèriaux et du Génie Physique, Grenoble INP, CNRS, Minatec, 3 parvis Louis Néel, 38016 Grenoble, France.

Resume : The mixed BaMgF4 (BMF) phase has recently attracted great attention due to its interesting multifunctional properties, such as room temperature piezoelectricity and ferroelectricity, transparency (<140 nm) and diamagnetic behavior. These properties offer great potential for application in electronic devices such as sensors, microactuators, infrared detectors, microwave phase filters, energy storage and non-volatile memories In the present study, a comparison between conventional and liquid injection metal-organic chemical vapor deposition (MOCVD) is reported and the relative synthetic routes for the growth of BaMgF4 on Si (001) and single crystalline SrTiO3 (001) substrate have been investigated. For the two used approaches, the volatile, thermally stable □-diketonate complexes Ba(hfa)2tetraglyme and Mg(hfa)2(diglyme)2(H2O)2 have been used as single precursors (C-MOCVD) or as solution multimetal source (LI-MOCVD). Structural and chemical characterizations through X-ray diffraction, transmission electron microscopy, energy dispersive X-ray and wavelength dispersive X-ray analyses confirmed the formation of pure, epitaxial BaMgF4 films on SrTiO3 substrates. Piezoresponce Force Microscopy has been used to asses piezoelectric properties. The impact of process parameters on film properties has been addressed, highlighting the strong influence of precursor composition, deposition temperature and oxygen partial pressure on the films composition, microstructure and morphology.

14:00

Atomic scale modeling of glassy chalcogenide surfaces: insights into their adsorption and gas separation properties

X.PII.40

Authors : G. Ori1, B. Coasne234, M. Boero1, C. Massobrio1
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Resume : Owing to their large surface area and tunable pore size, amorphous porous solids such as siliceous, carbonaceous and chalcogenide materials are at the heart of important applications: energy (H2 storage, lithium batteries) and environment (water treatment). Recently, nanoporous chalcogenides (chalcogel) have been demonstrated to be efficient sorbents for environmental remediation from gaseous and water waste media. From a computational point of view, producing glassy surface models capable of mimicking realistically the behavior of a chalcogel and its surface is mandatory in order to understand the structure and adsorption properties of such complex amorphous materials. In this contribution, first-principles and classical atomistic simulations are combined to study the properties of glassy chalcogenide surfaces. Several chemistries will be considered. First-principles molecular dynamics is used to develop a realistic model of these materials with special

emphasis on their surface chemistry. A detailed account of the structure of the surface models is given in terms of pair correlation functions, structure factors, chemical order and chemical bonding. The surface properties of these materials will then be assessed by simulating adsorption isotherms of various fluids using classical Monte Carlo simulations. I will show how the realistic details of the surface chemistry drastically affect the adsorption of various gases such as N2, CO2, CH4, H2 and their mixtures.

14:00 High-Quality VO2 Thin Film Nanostructures for Femtosecond Metal Insulating Transition (MIT) Optoelectronic Sensors and Smart Energy-Efficient Windows **X.PII.41**

Authors : M Saad1,2,3, M Millen1, A Kumar1, L Klien4, P Kozlowski4, M Gregg1
Affiliations : 1 Queens University Belfast, UK 2 Egypt Nanotechnology Center (EGNC), Cairo University, Egypt 3 Suez University, Egypt 4 IBM Watson Research Center, USA

Resume : Complex multifunctional oxides such as VO2 have attracted a huge R&D interest because of their ultrafast sharp metal insulating transition (MIT) with a significant change in the electrical resistance making them excellent candidates for a variety of next generation novel optoelectronic nanotechnology applications including femtosecond sensors, gas sensors, smart windows for energy-efficient buildings and information storage memories. A series of high quality VO2 thin film nanostructures were successfully grown on both Al2O3 single crystal substrates and RuO2 conducting oxide thin film buffered Al2O3 substrates using a Pulsed Laser Deposition (PLD) system. Conducting mapping of the MIT phase transition in the VO2 thin films at different temperatures using a PFM technique was discussed. Transport measurements of the VO2 epitaxial thin films on Al2O3 substrates as a function of temperature showed a sharp 1st order MIT phase transition with a huge and ultrafast change in the electrical resistance up to 4 orders of magnitude at a transition temperature of 68 +/- 3 C. Moreover, theoretical calculations of the VO2 thin films grown on RuO2 buffered Al2O3 substrates could successfully and perfectly recover the 1st order sharp MIT phase transition with significant change in resistivity as in bulk of the VO2 regardless the conducting oxide thin film underneath it.

15:30 *Coffee break*

START AT SUBJECT View All NUM. ADD

Nanomaterials for Optical Gas Sensing : Joan Daniel Prades

09:00 Luminescence Probing of Adsorption Phenomena on InGaN/GaN Nanowire Arrays **X.VIII.1**

Authors : Konrad Maier*, Andreas Helwig*, Gerhard Müller*,**, Jörg Teubert***, Martin Eickhoff***
Affiliations : * Airbus Group Innovations, D-81663 München, Germany; ** Munich University of Applied Sciences, Fachbereich 06, Lothstraße 34, D-80335 München, Germany; *** I. Physikalisches Institut, Justus-Liebig-Universität Gießen, D-35392 Gießen, Germany.

Resume : InGaN/GaN nanowire arrays exhibit an efficient photoluminescence (PL) which persists from 4K up to about 600K. As this PL is sensitive to the presence of adsorbates

on the InGaN surfaces, it is also a very useful probe for the investigation of adsorption phenomena. Unlike reducing gases (H2, hydrocarbons), which hardly induce any PL changes on bare InGaN surfaces, oxidising ones (O2, NO2, O3) efficiently quench the PL. At room temperature minimum detectable O3, NO2 and O2 concentrations are 5 ppb, 20 ppb and 400 ppm, respectively. H2O, on the other hand, which can exist in large and largely variable quantities in the ambient air, plays an interesting double role both as a quencher and as an enhancer of the native PL. An analysis of the PL changes in terms of our recently published Langmuir Adsorption and Recombination model, indicates that the Langmuir adsorption energy Eads remains very low (Eads ~ 0eV) up to 30-50K, and then increases linearly with temperature up to at least 400K. This behaviour indicates that all gases first physisorb and then start to settle down into more and more tightly bound chemisorption states as the InGaN temperature is raised. At room temperature Eads attains values between 0.4 and 0.8eV, increasing in the order H2O, O2, NO2, and O3. Due to their stronger binding NO2 and O3 adsorbates appear to displace pre-adsorbed O2 ones via a competitive adsorption process. H2O molecules, finally, appear to adsorb in at least two different forms, eventually forming multi-layer adsorbates, which can effectively absorb water-soluble gases (NO2, NH3) while disabling any direct surface interaction of non-water-soluble ones.

09:30 Plasmonic nanomaterials for sensing applications **X.VIII.2**

Authors : Rashad Hajimammadov, Krisztian Kordas
Affiliations : Microelectronics Research Unit, Faculty of Information Technology and Electrical Engineering, University of Oulu P.O. Box 4500, FI-90570 Oulu, Finland

Resume : We report on gas sensing with nanomaterials based on Cu nanowires and CuPd nanotube alloys as challenging alternatives to conventional plasmonic noble metal sensors. The metal nanowires and nanotubes are synthesized by solvothermal growth and subsequent galvanic replacement, respectively. The sensors based on the 1D nanomaterials are prepared by inkjet deposition between Pt electrodes lithographically defined on silicon chips. The change of the electrical conductivity is measured as a function of time, temperature, illumination, nanowire composition and concentration of harmful gases such as NH3 and CO. The assessment of the sensing behavior of the used materials showed a clear dependence on above mentioned factors, especially on the concentration of Pd in the 1D nanomaterials. Possessing a natural resist to oxidation in atmospheric ambient and low temperatures Pd significantly alters the electrical and sensing properties of the bimetallic nanowire, ensuring pure metallic behavior responsible for the plasmonic sensing.

09:45 Ellipsometric characterization of metal doped SnOx thin films for SPREE-based gas sensors **X.VIII.3**

Authors : Daniel Fischer (a), Andreas Hertwig (a), Uwe Beck (a), Martin Kormunda (b), Norbert Esser (c)
Affiliations : (a) BAM Federal Institute for Materials Research and Testing, Division 6.7, Unter den Eichen 87, 12205 Berlin, Germany; (b) J.E. Purkyne University, Faculty of Science, Department of Physics, Ceske mladeze 8, 400 96 Usti nad Labem, Czech Republic; (c) Leibniz Institut für Analytische Wissenschaften ISAS-e.V., Department Berlin, Schwarzschildstr. 12, 12489 Berlin, Germany

Resume : Gas sensors are an important tool in various areas for example in industrial process control, as well as security applications or in research. In this study, a noninvasive gas detection technique, based on the SPR effect with ellipsometric readout (Surface Plasmon Resonance Enhanced Ellipsometry-SPREE), is investigated. The gas sensor consists of a 40 nm SPR-active gold layer and a top-coated 5 nm doped SnOx layer. In the past, it could be shown that, without the top-coating, these type of sensors can detect various gases with sensitivities down to the ppm range (in air). The goal of the present study is to characterize additional top-coating materials (mainly doped SnOx) in dependence of the coating conditions. With the help of the doped-metal oxide, the sensitivity increases by two order of magnitude. Additionally, a selectivity for specific gases (e.g. CO for Fe-doping) is observed which depends on the doping conditions of the coating. Changing the properties of the plasma coating process gives access to a big variety of different layers and enables us to find the best conditions for the determined gas in selectivity and sensitivity. The result of the sputtering progress is analyzed and characterized by using optical methods, mainly spectroscopic ellipsometry (SE), as well as TOF-SIMS, TEM and AFM to find a correlation between the doping concentration, surface structure, the optical properties and the resulting sensing ability.

10:00 *Coffee break*

Hybrid Materials for Environmental Sensing : Danick Briand

10:30 ADVANCED HYBRID MATERIALS FOR ENVIRONMENTAL SENSORS **X.IX.1**

Authors : M. Bouvet, J.-M. Suisse, R. Meunier-Prest
Affiliations : Institut de Chimie Moléculaire de l'Université de Bourgogne, Univ. Bourgogne Franche-Comté, Dijon, FRANCE

Resume : Interest in molecular materials has been driven in large part by their various and prosperous applications, especially in the domain of organic electronics, where they offer many advantages as well as alternative approaches. In the present review, we show how the chemical variability of phthalocyanines allowed synthesizing a broad range of hybrid materials. The combination of phthalocyanines or related derivatives with polymers or carbonaceous materials led to efficient chemical sensors. It is shown how the incorporation of macrocyclic molecules in hybrid materials highly modifies the structural and morphological characteristics of the materials. Rugosity, specific surface and porosity being key parameters in the analyte-sensing material interactions, these modifications highly improve the performance of chemical sensors. This is the reason why they are particularly promising materials for the development of new chemical sensors, associated with electrochemical, conductometric or optical transducers. We will show mainly two types of sensing materials, firstly phthalocyanine – grafted carbon nanotubes (CNTs), secondly conducting polymer – phthalocyanine hybrid materials. The combination of phthalocyanines and porphyrins with carbonaceous materials or with polymers in hybrid materials offers the possibility to tune their physical properties, leading to chemical sensors with better performances compared to these prepared from a single component. In addition, these hybrid materials can be deposited, at room temperature, by solution processing.

11:00 Composite Structure Based on Graphene Oxide **X.IX.2**

and Metal Oxide Nanomaterials for Chemical Sensors.

Authors : Vardan Galstyan, Elisabetta Comini, Iskandar Kholmanov, Andrea ponzoni, Veronica Sberveglieri, Nicola Poli, Mona Mirmotallebi, Guido Faglia, Giorgio Sberveglieri
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Resume : Chemical gas sensors based on metal oxides are among the most used devices for the detection of the gas during the environmental, safety and food quality monitoring. ZnO is one of the widely investigated structures for gas sensing due to its high thermal/chemical stability. The sensing mechanism of ZnO chemical sensor is based on the variation of its electrical conductivity in the presence of gases. The studies showed that the ZnO has high sensitivity mainly towards ethanol or acetone. Detection of other gases, such as CH4, NO2, and H2, is of vital interest for wide range of applications. Therefore, the improvement of sensing performance of ZnO for the detection of these toxic, explosive and hazardous gases is remaining as a challenging issue. Graphene and modified graphene were studied for application in gas sensors. The studies showed that the graphene and its oxides might be used as new additives in composite materials for gas sensors. In our work, we report fabrication of a graphene oxide/ZnO composite by coupling graphene oxide (GO) and ZnO nanostructures. We obtained ZnO nanostructures by electrochemical anodization and thermal annealing. Graphite oxide was produced from natural graphite using a modified Hummers method. Aqueous dispersion of GO was prepared by stirring graphite oxide solids in pure water, and then sonicating the resulting mixture for 45 minutes. The fabricated nanocomposites were tested as a sensing material for detection of NO2, H2 and CH4 gases. We found out that the reducing the GO enhanced the nanocomposite conductance and improved the response of composite to all measured gases. The obtained results showed that the fabricated nanocomposite material is promising for development of chemical sensors and electronic noses.

11:15 Electronic ammonia sensor based on hybrid polyaniline/metal oxides nanocomposites **X.IX.3**

Authors : S. Mikhaylov*,**, J-L. Wojkiewicz*, A. Pud**, N. Ogurtsov**, Yu. Noskov2** N. Redon*, P. Coddeville*
Affiliations : * Ecole des Mines-Douai, Atmospheric Science and Environment Engineering, F-59508 Douai, France ** Institute of Bioorganic Chemistry and Petrochemistry, National Academy of Sciences of Ukraine, 50 Kharkivske

Shose,02160, Kyiv, Ukraine

Resume : In regards to its wide use, global ammonia emission in atmosphere increases continuously since the pre-industrial times promoting the formation of particulate matter and affecting flora, fauna and the quality of air and now ammonia is becoming a major pollutant. The main sources of ammonia come from agriculture (fertilizers), animal waste fermentation and industry (refrigeration units…). Ammonia has adverse health effects as respiratory disorder; skin irritation, severe irritation at the ocular level, nausea, headache and an exposition to high concentrations can be fatal. In working places, ammonia concentration is regulated. Moreover ammonia is subject to produce odor nuisances with a negative impact in terms of the quality of life of citizens, safety and economy. In regards to its toxicity, its detection is of great importance for environment. This is why we created new ultra low cost organic electronic gas sensors based on hybrid nanocomposites with metrological performances adaptable to the application. These hybrids based on an intrinsically conducting polymer (polyaniline) and metal oxides (TiO2, SnO2) exhibit synergistic effect due to specific chemical and physical interactions along their interfaces in the composite. Our work was directed on influence estimation of two surface active acids i.e. dodecylbenzenesulfonic acid (DBSA) and lauryl sulfuric acid (LSA) on PANI nanocomposites structure-property relationship and effects of nanoparticles on aniline polymerization kinetics. These effects were used to to optimize the response of the sensors to get linear response in the ppm range or/and to get low detection threshold. The detection threshold can be adapted from ppb to ppm values with response times around one minute. As these sensors are processed in solution, they can be printed on adequate substrates to get miniaturized sensors to create dense sensor networks for environment monitoring.

11:30 Semiconducting 2D materials for highly sensitive sensing **X.IX.4**

Authors : Torben Daeneke Kourosh Kalantar-Zadeh
Affiliations : School of Engineering, RMIT University; School of Engineering, RMIT University

Resume : Two dimensional (2D) materials such as atomically thin transition metal oxides and chalcogenides are an excellent platform for sensing applications due to their extraordinary surface area to volume ratio. This morphology allows surface bound analytes to effectively interact with the highly confined and comparatively small number of charge carriers in the 2D system leading to highly sensitive sensing. Analogous to graphene, stratified transition meatal oxides and chalcogenides (TMO&S) can be exfoliated to their unit cell thick fundamental layers with relative ease; however unlike graphene many TMO&S feature a bandgap which can be exploited for the sensing process either via the modulation of photoluminescence arising from a direct bandgap or through the modulation of the electronic structure of the material which can be electronically detected. Furthermore intercalation of multilayer TMO&S with small cations (H+, Li+ etc) has been found to effectively dope the 2D materials, leading to plasmon resonances in the visible spectrum. Surface interaction with an analyte can then further perturbatie the electronic structure of the intercalated 2D material generating an optical signal which can be easily detected. Different sensors based on native and intercalated semiconducting 2D materials will be discussed herein.

11:45 Au@Cu2O Core-Shell Nanocrystals Exhibited Remarkable Peroxidase-like Catalytic Activity **X.IX.5**

Authors : Ming-Yu Kuo and Yung-Jung Hsu*
Affiliations : Department of Materials Science and Engineering, National Chiao Tung University, Hsinchu, Taiwan.

Resume : Au nanoparticles have been found to show potentials for various applications such as catalysis, biomedicine, gas sensing, etc. Among the different catalysis applications, Au nanoparticles as artificial enzyme to perform a myriad of oxidation reactions may pose significant implications in both materials science and biomedicine aspects. However, plain, un-modified Au nanoparticles are prone to aggregation during the catalytic reactions, which further hinders their practical use. To address this issue, core-shell structures in which Au nanoparticles are coated with a thin layer of shell material are proposed. For core-shell structures, the core Au particles are protected by the shell material from being aggregated during the reaction period. On the other hand, each of the Au can participate in the catalytic reaction, providing a homogeneous reaction environment to facilitate the catalysis. In this study, Au@Cu2O core-shell nanocrystals have been synthesized and demonstrated remarkable enzyme-mimetic activity toward H2O2 decomposition. The peroxidase-like activity of Au@Cu2O was evaluated by using tetramethylbenzidine (TMB) as the substrate in the presence of H2O2. The oxidation processes of TMB by using Au@Cu2O were analyzed with the typical Michaelis-Menten kinetics model, in which the Michaelis constant (Km) and maximum reaction velocity (Vmax) were obtained and compared. The influence of shell thickness on the activity of the samples were also investigated and realized.

12:00 Strategies for Low Power Gas Sensor **X.IX.6**

Authors : O. Monereo, N. Markiewicz, J. Samà, O. Casals, C. Fàbrega, F. Hernandez-Ramírez, A. Cirera, A. Romano-Rodríguez, A. Waag, J.D. Prades
Affiliations : MIND/IN2UB, Departament d'Electrònica, Universitat de Barcelona, Spain Institute for Semiconductor Technology, Braunschweig University of Technology, Germany

Resume : The energy needed to activate the chemical processes occurring at the surface of solid-state sensor materials is the main source of power consumption of this technology. In this presentation, we will review recent advancements in thermal and optical methods to supply such energy in an efficient way. On the one hand, self-heating in nanostructures is a promising but barely unexploited approach to reduce power consumption under the tens of µW regime. The technical complexity of fabricating suitable devices for such approach has hampered its further development for nearly a decade. Recent results show that efficient self-heating also occurs on larger systems, which are simpler to fabricate. Moreover, new findings about the origin of the unexpected efficiency of these large systems are opening doors for truly engineering self-heated devices easy to implement. On the other hand, optically activated conductometric devices have remained dormant as a scientific curiosity over the years. Most of the past limitations came from the need of UV light sources of relatively high costs. Advancements in LED technology extended the flexibility of the LED technology in the last years, at a much lower cost. In parallel, materials modifications and surface functionalization strategies relaxed the need of UV, making possible the use of other, more efficient and convenient, wavelengths (e.g. visible blue). On top of that, optical activation approaches conductometric operation to the world

of optoelectronic, in which further power savings can be achieved (e.g. zero power operation) by using active sensor structures.

12:30 *Lunch*

Advanced Transducers for Chemical Sensing : Anita Lloyd Spetz

14:00 GaN based sensor for ultra-low-power air quality monitoring **X.X.1**

Authors : Peter Offermans, Ahmed Si-Ali, Greja Brom-Verheyden and Rob van Schaijk
Affiliations : imec/Holst Centre High Tech Campus 31 5656AE Eindhoven the Netherlands

Resume : A novel gas sensor platform based on AlGaN/GaN is developed for ultra-low-power air quality monitoring. Device fabrication is based on 8 inch GaN-on-Si wafers using a modified power-HEMT process, incorporating recessed open gate sensing areas and an integrated resistive heater structure. Due to the gate area recessing (to ~7nm AlGaN thickness), the device shows excellent sensitivity to NO2, a major air pollutant, allowing the detection of single-ppb steps in the gas concentration. The sensing mechanism is based on interaction of electron donating and withdrawing gases with surface states, resulting in a change in surface potential. A key advantage of the present device compared to state-of-the-art conductive metal oxide sensors is the small interference from humidity (<10% of the NO2 response). The NO2 sensor will also be integrated on a multi sensor platform developed in a FP7 EU project (MSP FP7 project 61187). The sensor is also used in control of a home air purification system in another EU project (ENIAC JU ESEE Project 324284). The response time of the sensor is strongly improved at higher operation temperature and for 250°C it is in the order of one minute. To minimize power consumption, suspended AlGaN/GaN membranes and beams were designed and optimized, enabling ultra-low-power heating with power consumption below 80 mW. Further decrease in power consumption is possible with smaller sensor areas and duty cycling. The platform can be extended towards other gases by surface functionalization. Surface modification was done by depositing Pt on the gate area for detection of H2 and with a 150nm thick polymer layer (PEI) for detection of CO2, both at ppm level.

14:15 Air Quality Networks- where do we go from here? **X.X.2**

Authors : John Saffell, Alphasense Ltd Great Notley, Essex CM77 7AA UK Roderic Jones, Dept of Chemistry, University of Cambridge CB2 1EW UK
Affiliations : Dr John Saffell, Alphasense Ltd Great Notley, Essex CM77 7AA UK Professor Roderic Jones, Dept of Chemistry, University of Cambridge CB2 1EW UK

Resume : Urban centres will need to monitor air quality using low cost air quality networks and costs are now affordable, but we now must resolve the details: deployment, maintenance, validation and data analysis. Monitoring gases, VOCs and particulates is difficult, but achievable. And air quality networks can be fixed site, car/tram mobile, personal and eventually wearable. Each network has opportunities and problems; calibration, data richness, political issues, personal data security must all be considered. Are the sensors providing good data? As requirements have moved from physical sensor networks (temperature, pressure, strain, light,

noise) to chemical sensor networks, the problems of data errors have increased. We will review progress in both North America and Europe on validation of air quality networks.

14:30 Method for field calibration of gas sensors **X.X.3**

Authors : Caroline Schultealbert, Tobias Baur, Andreas Schütze, Tilman Sauerwald
Affiliations : Lab for Measurement Technology, Saarland University, Saarbrücken, Germany;Lab for Measurement Technology, Saarland University, Saarbrücken, Germany;Lab for Measurement Technology, Saarland University, Saarbrücken, Germany;Lab for Measurement Technology, Saarland University, Saarbrücken, Germany

Resume : Gas sensor systems are inexpensive devices for measuring VOCs. However, adequate low cost methods for (re)calibration in the field are not available. To this end, a method based on the thermodynamic equilibrium of a 2-phase system by solving VOCs in a non-volatile liquid is developed. The vapour pressure of VOCs, and hence the concentration, in the headspace is modelled depending on the mole fraction (UNIFAC model). Exposing a sensor the headspace can be used for quick and inexpensive calibration. We show that squalane can be used as non-volatile liquid after a special cleaning procedure with nitrogen. The headspace of pure squalane can also be used as zero air standard, since VOCs have a partition coefficient of more than 2500 leaving the headspace almost VOC free under elsewise unchanged background conditions such as humidity and permanent gases. Calibration standards containing 10 ppb to 700 ppm toluene were produced, tested and compared to standards obtained by a gas mixing system. The headspace concentrations have as well been tested with GC-MS analysis. The method is demonstrated for the field calibration of sensor systems using a SnO2 gas sensor in temperature cycled operation. Those sensor systems use a special model based quantification method which shows better drift properties and the possibility to compensate background. Using the recorded calibration curve tests in indoor air were conducted proving a correct quantification under changing background conditions.

14:45 Optimization of the Field Effect Transistor transducer platform for the development of air quality sensors **X.X.4**

Authors : Mike Andersson, Manuel Bastuck, Joni Huotari, Donatella Puglisi, Andreas Schütze, Jyrki Lappalainen, Anita Lloyd Spetz
Affiliations : Div. of Applied Sensor Science, Linköping University, SE-581 83 Linköping, Sweden; Lab for Measurement Technology, Department of Mechatronics, Saarland University, Campus A5.1, DE-661 23 Saarbruecken, Germany; Microelectronics and Materials Physics Laboratories, Department of Electrical Engineering, University of Oulu, Linnanmaa, P.O.Box 4500, FIN-900 14 Oulu, Finland; Div. of Applied Sensor Science, Linköping University, SE-581 83 Linköping, Sweden; Lab for Measurement Technology, Department of Mechatronics, Saarland University, Campus A5.1, DE-661 23 Saarbruecken, Germany; Microelectronics and Materials Physics Laboratories, Department of Electrical Engineering, University of Oulu, Linnanmaa, P.O.Box 4500, FIN-900 14 Oulu, Finland; Div. of Applied Sensor Science, Linköping University, SE-581 83 Linköping, Sweden;

Resume : Following increased awareness of the adverse health effects caused by exposure to even trace amounts of certain air pollutants, the research and commercialization of

cost efficient means for highly sensitive, rapid, and reliable monitoring of such pollutants at ultra-low concentrations have attracted increased attention over the latest decades. A vast number of gas sensitive materials of different structure have been processed and characterized over this period, exhibiting different benefits for the detection of various substances. Considering the application of these materials in and their possible interaction with some transducer element, the final sensor performance is, however, also dependent on the characteristics of the transducer platform. Here is thus reported on investigations into the influence of transducer design and operation on its performance, e.g. sensitivity, response time, and reliability, as exemplified through the optimization of the Field Effect transducer platform for the development of air quality sensors. FET devices of different types and designs have been fabricated, employing some different materials for different parts, and characterized in different operational modes. From the findings it has for instance been concluded that depletion type devices with certain insulator materials and thicknesses operated in the saturation regime exhibit almost twice the sensitivity and orders of magnitude better stability than many other options.

15:00 Gas Sensors on Printed Flexible Substrates for Wearable Applications **X.X.5**

Authors : Danick Briand et al.
Affiliations : Ecole Polytechnique Fédérale de Lausanne (EPFL) Neuchâtel, Switzerland

Resume : We report in this communication on various environmental sensors fabricated on flexible substrates using printing technologies. We have developed a set of sensors working with different principles, capacitive, resistive, colorimetric, and field-effect. These transducers on polymeric or cellulosic substrates were functionalized with various sensing films (polymers and metal-oxides) using printing techniques. Different sensing devices operating at low power or with heating capability for sensing humidity, volatile organic compounds, reducing and oxidizing gases have been produced and evaluated. Formation of arrays has also been investigated and multi-sensor platforms were demonstrated. Performance vs. cost, status and current trends on printed environmental sensors will be discussed. Finally, examples of systems involving these sensors will be described, notably smart RFID labels and smart textiles.

15:30 *Coffee break*

Functional Materials for New Sensor Concepts : Katarzyna Zakrzewska

16:00 Suspended SWNT in FETs as Functional Material for Ultra Low Power NO2 Sensors **X.XI.1**

Authors : Christofer Hierold, Kiran Chikkadi, Cosmin Roman, Miro Haluska
Affiliations : ETH Zurich, Micro and Nanosystems, Department of Mechanical and Process Engineering, CH-8092 Zurich

Resume : We report on the concept of applying single walled carbon nanotube field effect transistors (SWNT FETs) as functional building blocks in sensors [1]. Advances in fabrication processes as well as better understanding of the behavior of SWNT FETs has enabled the vision of using individual-tube devices directly for NO2 gas sensors. Significant progress has been made in understanding the

sources of noise, drift and hysteresis, and techniques have been introduced to counteract them, such as pulsed measurements and suspended device architectures. Reducing the presence of process residues and dielectrics close to the SWNT to the best possible level leads to the suppression of hysteresis and significant improvement in the noise performance [2,3,4], as well as improvement in the cross-sensitivity to humidity. Suspended devices are also attractive for self-heated, low-power architectures [5]. We will discuss the influence of different options of device architectures and integration and process flows on the device performance with a focus on hysteresis, noise and ultra low power sensing. With improving control over fabrication processes gas sensor functional devices operating at extremely low power can be envisioned. In this respect, suspended, self-heated gas sensors appear to be the preferred architecture also due to the low-power recovery and low noise performance. Acknowledgments: Matthias Muoth, Wei Liu, Moritz Mattmann, Laura Jenni, Lalit Kumar and Sebastian Eberle for their contributions to SWNT-FET NO_2 sensors, Support from ETH Zurich (TH 18/03-1, TH 13/05-3), Swiss National Science Foundation (20021-108059/1 and 200021_153292/1) and KTI/CTI (8885.2 PFDP-NM) is gratefully acknowledged. References: [1] Hierold, C.; Jungen, A.; Stampfer, C.; Helbling, T., Sens. Actuators, A 2007, 136, pp 51 [2] Chikkadi, K.; Muoth, M.; Roman, C.; Haluska, M.; Hierold, C., Beilstein Journal of Nanotechnology, 2014, 5, pp 2179 [3] Chikkadi, K.; Muoth, M.; Liu, W.; Maiwald, V.; Hierold, C., Sens. Actuators, B 2014, 196, pp 682 [4] Liu, W; Chikkadi, K; Lee S-W.; Hierold, C.; Haluska, M; Sens. Actuators B 2014, 198, pp 479 [5] Chikkadi, K.; Muoth, M.; Maiwald, V.; Roman, C.; Hierold, C., Appl. Phys. Lett. 2013, 103, pp 223109

16:30 Self-Supported Three-Dimensionally Interconnected Polypyrrole Nanotubes and Nanowires for Highly-Sensitive Gas Detection **X.XI.2**

Authors : Vlad-Andrei Antohe (a), Etienne Ferain (b), Driss Lahem (c), and Luc Piraux (a);
Affiliations : (a) Institute of Condensed Matter and Nanosciences (ICMN), Université catholique de Louvain (UCL), Place Croix du Sud 1, 1348 Louvain-la-Neuve, Belgium; (b) it4ip s.a., Avenue Jean-Etienne Lenoir 1, 1348 Louvain-la-Neuve, Belgium; (c) Materia Nova, Materials R&D Center, Avenue Nicolas Copernic 1, 7000 Mons, Belgium

Resume : Three-dimensional networks made up of nanowires or nanotubes are expected to play an important role in the development of next generation of nanostructured devices, as the high degree of wire/tube interconnectivity may be beneficial in a wide range of applications, including chemiresistive sensing. Specifically, we report a novel and reliable method to fabricate highly-sensitive environmental chemiresistive gas sensors based on large-scale interconnected networks of electroconductive polymer nanotubes. The versatile bottom-up strategy allows facile fabrication of centimeter-scale free-standing arrays of interconnected polypyrrole nanotubes (or nanowires) with tunable geometrical dimensions and spatial arrangement. Such networks of elongated nanostructures have great potential to be used in sensing applications, as they provide an extremely large active surface, together with remarkable electrical connectivity and mechanical stability. In particular, the scalable three-dimensional system of polypyrrole nanotubes exhibits an excellent sensitivity toward gaseous ammonia, at gas concentrations as low as 1 ppm. It’s worth pointing out that the entire sensor’s fabrication protocol is exclusively based on simple and low-cost technologies with no sophisticated processing steps, such as lithographic approaches. The as-prepared sensors based on these dense

hierarchical nanoarchitectures may be therefore easily integrable for specific and highly-sensitive detection of several gas species.

16:45 Supramolecular Approach for the Detection Benzene in Air at ppb Level **X.XI.3**

Authors : R. Pinalli (a), E. Dalcanale (a), S. Zampolli (b)
Affiliations : (a) Department of Chemistry, University of Parma, 43124 Parma, Italy (b) CNR - IMM Bologna, 40129 Bologna, Italy

Resume : The need of fast, sensitive and accurate real time analyses is the driving force for the development of sensor technology. Environmental air quality monitoring is generally executed using complex and expansive instruments, based on laboratory equipment adapted to in-field use. While low-cost devices for real-time monitoring of CO, NOx and O3 are available, aromatic hydrocarbons like benzene, toluene and xylenes (BTX) are generally still monitored with passive samplers and successively off-line analyzed, resulting on data representing averaged exposure levels. In order to provide significant air quality data, reliable quantification of single BTX must be performed. We already reported on a miniaturized system able to reach this goal [1, 2]. Here the results of new efforts aiming to further simplify the system, maintaining the reliability of the data, are presented. A miniaturized system is proposed, composed of a selective supramolecular concentration unit, a MEMS cartridge, filled with the supramolecular cavitand receptor, and a commercial PID as sensor. The issue of achieving at the same time molecular-level selectivity and low-ppb sensitivity for benzene has been solved by disconnecting the recognition element from the detection unit. The recognition event is assigned to a molecular receptor, capable of selectively trapping aromatic vapors at the gas–solid interface. The MEMS cartridge can be heated with a precise control of temperature; the cavitands selectively release species in function of temperature. In this way the MEMS cartridge works as a trap of aromatics compounds at room temperature, and as a GC-like column when heated. [1] Dalcanale E. et al. Chem. Comm. 2007, 2790. [2] Dalcanale E. et al. Sens. Act. B 2009, 141, 322.

17:00 Fully solution-processed OFET platform for gas sensing applications **X.XI.4**

Authors : E. Danesh (a), S. Faraji (b), D. J. Tate (c), K. C. Persaud (a), L. A. Majewski (b), S. G. Yeates (c), M. L. Turner (c)
Affiliations : (a) School of Chemical Engineering & Analytical Science, The University of Manchester, Manchester, M13 9PL, UK; (b) School of Electrical & Electronic Engineering, The University of Manchester, Manchester, M13 9PL, UK; (c) School of Chemistry, The University of Manchester, Manchester, M13 9PL, UK

Resume : This report describes the development of a gas sensor array based on low-temperature, all solution-processed bottom-gate bottom contact organic field-effect transistors (OFETs) that operate at low voltages (~2 V). Gate electrodes (width 200 µm) were patterned on a PEN substrate from a commercial silver nanoparticle-based ink using a Dimatix DMP-2831 inkjet printer, and sintered at 120 C. The gate electrodes were coated with a high-k/low-k bilayer gate dielectric. Source and drain electrodes were inkjet printed to produce a channel width and length of 2 mm and ~100 µm, respectively. Poly(3,6-di(2-thien-5-yl)-2,5-di(2-octyldodecyl)-pyrrolo[3,4-c]pyrrole-1,4-dione)thieno[3,2-b]thiophene)

(DPPTTT) was used as the active layer of the sensing array. The system was developed for sensing ammonia due to its relevance for environmental and health monitoring applications. The response of the sensor was monitored as the change in the OFET's source-drain current upon exposure to various concentrations of ammonia. DPPTTT-based sensors showed rapid, sensitive and reversible room temperature response to ammonia vapour both in dry and humid air (relative humidity = 20 – 80%) over the concentration range of 1-50 ppmv. The results demonstrated here further illustrate the potential of these OFET arrays in novel printed electronics applications, such as low-cost and low-power flexible sensors.

17:15 GaAs as a sensitive material in acoustic gas sensor **X.XI.5**

Authors : G. Bailly, J. Rossignol, Th. Leblois
Affiliations : ICB, CNRS UMR 5209, UBFC, 9 avenue Alain Savary 21078 Dijon, France; ICB, CNRS UMR 5209, UBFC, 9 avenue Alain Savary 21078 Dijon, France; FEMTO-ST Institute, CNRS UMR 6174, UBFC, 15B avenue des Montboucons 25030 Besançon, France

Resume : The piezoelectric sensors are known for their high accuracy, low manufacturing cost and high level of miniaturisation. Moreover, GaAs is a crystal with a lot of interesting properties for MEMS applications such as piezoelectric properties, microfabrication opportunities and various possibilities to biofunctionnalize its surface to reach the specificity of molecules grafting. These three points have given us the opportunity to develop a specific GaAs acoustic sensor adapted for detection of molecules in specific media. Using analytical model, we showed that the best performance for electromechanical coupling is obtained in a (100) wafer with an electric field aligned along the <110> direction. The transducer whose active structure is a membrane was obtained using low cost processes of microfabrication and then was connected to PCB to be characterized. The results given here concern the S parameters of the device in wideband frequency (15MHz to 1GHz), microwave microscopy of the electromagnetic field repartition on the sensitive surface. These characterizations constituted preliminary results to optimize the design of electrodes before measurements in gas environment. We have evaluated of the microwave transduction with GaAs in argon flux. The polluant species are toluene and NH3. The interactions between the sensitive material and the gas are demonstrated. The observed variation of the sensor response is clearly due to the variation of the adsorption of gas.

17:30 Modification of the chemical and electronic properties of n-type GaN(0001) surfaces by potassium and water adsorption **X.XI.6**

Authors : V. Irkha, A. Eisenhardt, S. Reiß, S. Krischok, M. Himmerlich
Affiliations : Institut für Physik and Institut für Mikro- und Nanotechnologien MacroNano, Technische Universität Ilmenau, Germany

Resume : GaN-capped open gate AlGaN/GaN based HEMTs are used for sensing pH values and ion concentrations in liquids. One example is the monitoring of cell metabolism processes via exchange of potassium ions in a bioreactor. In order to characterize the processes during potassium and water interaction with the HEMT surface, we have investigated their adsorption at n-type GaN(0001) surfaces at 300 K using in-situ photoelectron spectroscopy with focus on adsorbate-substrate charge transfer processes. K adsorption and K &

H2O coadsorption initially lead to the saturation of surface dangling bonds accompanied with drastic changes in the interface properties. In all cases, a strong surface dipole forms, lowering the electron emission barrier. Two reaction regimes are identified, which mainly depend on the K coverage. The initial stages are characterized by K ionization and transfer of the 4s electrons towards the substrate inducing an increase of the GaN surface electron density. For higher K coverage, the residual 4s electron density induces the formation of intra-gap states and recovery of surface electron depletion. In case of water interaction, hydroxyl groups are formed including creation of flat band conditions at the GaN surface. The surface band alignment varies between 0.5 eV upward band bending and -0.5 eV downward bending clearly demonstrating that the electron density at the GaN surface can be reversibly tuned by alkali-based adlayers depending on their nature and thickness.

17:45 Molecular understanding of catalyst as sensor: an in situ impedance-DRIFT spectroscopy study of NH3-SCR reaction on zeolites **X.XI.7**

Authors : Peirong Chen, Simon Schönebaum, Dieter Rauch, Ralf Moos, Ulrich Simon
Affiliations : RWTH Aachen University; RWTH Aachen University; University of Bayreuth; University of Bayreuth; RWTH Aachen University

Resume : Selective catalytic reduction of nitrogen oxides (NOx) by NH3 (NH3-SCR) is one of the most promising strategies for the abatement of NOx emissions from diesel engines. To further improve the efficiency of NH3-SCR, it is necessary to get insights into the real-time state of the applied catalysts (mostly zeolite-based) under operational conditions. As revealed in our previous studies by impedance spectroscopy (IS), the proton transport in H-ZSM-5 was supported by stored NH3 as a solvate molecule, which allows H-ZSM-5 zeolites to be used in the sensing of both gas-phase NH3 and NH3-SCR reactions. Here, we performed in situ IS studies on highly comparable zeolites Fe-ZSM-5 and Cu-ZSM-5 (with the Cu or Fe species predominantly in isolated state) as catalysts and sensors simultaneously under SCR-related conditions. While the SCR conversion of stored NH3 on Fe-ZSM-5 can be effectively monitored based on NH3-supported proton transport, the sensing of SCR conversion of stored NH3 on Cu-ZSM-5 was significantly influenced by the formation of intermediates. Simultaneous IS and DRIFTS (diffuse reflection infrared Fourier transform spectroscopy) studies revealed that ammonium ions formed immediately by exposing NH3-saturated Cu-ZSM-5 to NO-containing atmospheres, and subsequently dominated the proton conductivity. Such a correlation of integral electrical response with molecular processes, achieved by our IS-DRIFTS studies, not only clarifies the molecular origin of the NH3-SCR sensing effect, but also provides a new perspective to understand the NH3-SCR mechanism over metal-promoted zeolites.

18:00 Self-Healable, Fully-Functional and Multiparametric Flexible Sensing Platform **X.XI.8**

Authors : Tan-Phat Huynh and Hossam Haick
Affiliations : The Department of Chemical Engineering and Russell Berrie Nanotechnology Institute, Technion – Israel Institute of Technology, Haifa 3200003, Israel

Resume : The implementation of flexible sensors in real-world applications calls for self-healing properties in similar way to the human skin. We present here a non-biological and flexible

self-healing platform that is sensitive to pressure, temperature, and gas analytes. For demonstration, we describe the fabrication of a complete self-healing device in the form of a bendable and stretchable chemiresistor, in which every part of this sensor is self-healing. The device has high sensitivity to pressure and strain highly comparable to other technologies. Moreover, the same self-healing platform is sensitive to both polar and apolar volatile organic compounds with a detection limit of 20 ppb. This self-healing device can be adapted, upon small changes in the architecture, to temperature with very high resolutions. Advantageously, analyte, temperature and pressure sensitivity is stable under multi-cycles of cutting/healing. This self-healing sensor increases the possibility that flexible devices might one day become self-administered, thus increasing their reliability in diverse applications in environmental sustainability and energy efficiency of the urban life.

START AT	SUBJECT	View All	NUM.	ADD

Environmental Sensor Technologies : Christofer Hierold

09:00 **Optical sensing of bio-medical targets using complex 3D nano-architectures** **X.XII.1**

Authors : S.H. Christiansen, G.Sarau, S.W. Schmitt, L. Kling, C. Tessarek, M. Latzel, Ch. Daniel, K. Amann
Affiliations : Helmholtz-Zentrum Berlin, Institute of Nano-architectures for Energy Conversion; Max-Planck-Instiute for the Science of Light, Erlangen

Resume : Complex nano-architectures of various material combinations (e.g. Si-nanostructures such as wires (NW) and cones (NC), GaN nanostructures, transparent conductive oxides e.g. Al doped ZnO, coinage metal nanoparticles e.g. wires, spheres, graphene and other 2D materials) integrated on Si wafer platforms will be presented to enhance selective optical sensing applications. Among those we show nano-material choices for surface enhanced Raman spectroscopy (SERS) and chemically functionalized resonators such as SiNWs, SiNCs, GaN NWs with distinct resonances for which peak shifts can be determined and quantitatively evaluated based on numerical simulations. We show for selected examples of interest in the area of bio-medical research our nano-material choices, the synthesis options and the viability to serve as signal enhancing SERS substrates. To understand optical signatures with respect to spectral analyte outputs, finite difference time domain (FDTD) simulations are carried out based on which 3D material architectures as signal enhancing substrates will be optimized. Bio-medical targets are from the field of kidney diseases and -injuries as well as bone degradation.

09:30 **Multiple Fe2O3-interlayered NiO with vertically ordered nanostructure for highly sensitive and selective VOCs gas sensor** **X.XII.2**

Authors : Jun Min Suh1, Young-seok Shim1,2, Ho Won Jang1,*
Affiliations : 1. Department of Materials Science and Engineering, Seoul National University, Seoul 151-744, Republic of Korea; 2. Department of Materials Science and Engineering, Yonsei University, Seoul 120-749, Republic of Korea

Resume : In recent days, there have been increasing attentions toward internet of things (IoT) and one of the emerging research area on IoT is about gas sensors to detect harmful agents that have high potential of causing damages to human body. Especially, volatile organic compounds (VOCs) which are very common in our ordinary life can cause serious damages. Therefore, gas sensors to detect and monitor VOCs have been studied for last decades. Among them, metal oxide semiconductor showed simple operation, cost-effectiveness and fast gas sensing performance with small-scale available, just suitable for IoT application. However, there still remain several challenges like reproducibility for mass production, better selectivity and response time. We present a simple method to solve existing problems through vertically ordered NiO nanorods with

Fe deposited in multiple steps by glancing angle deposition. The highly ordered porous structure with multiple p-n junctions of NiO and Fe2O3 formed after annealing at air ambient showed dramatically enhanced response to volatile reducing gases (C2H5OH, C7H8, C6H6, CH3COCH3 and CH3CHO) with fast response time (< 5s) compared with bare NiO nanorods. Interestingly, NiO with Fe2O3 reacted differently to target gases, leading to selective detection. These results are attributed to p-n junctions for response increase (transducer function), effective structure for better gas accessibility (utility factor), and catalytic effect of Fe2O3 (receptor function).

09:45 The European Sensor Systems Cluster - ESSC: A Tool for Implementing EC Clustering Policies on Sensor Technologies **X.XII.3**

Authors : Michele Penza - on behalf of ESSC Cluster
Affiliations : ENEA, Italian National Agency for New Technologies, Energy and Sustainable Economic Development Lab Functional Materials and Technologies for Sustainable Applications - PO Box 51 Br4; I-72100 Brindisi, ITALY

Resume : This is a is a short overview of the European Sensor Systems Cluster (ESSC), that is an EC initiative, launched on November 2014, to maximize impact of the FP7/H2020 research and innovation projects for industrial leadership and key enabling technologies applications. The ESSC cluster has already involved 7 FP7/H2020 projects, European networks and platforms, 13 founder organizations with at least 60 members from more than 15 Countries (January 2016). The European Commission launched a new initiative in the field of Research & Innovation with European Clusters to promote international cooperation, create critical mass in Science & Technology and maximize impact in strategic key sectors for European economic growth with high industrial relevance. The European Sensor Systems Cluster (ESSC) (http://www.cluster-essc.eu) was launched in Brussels on 27 November 2014 under sponsorship of the DG Research and Innovation, Directorate Key Enabling Technologies - Unit Advanced Materials and Nanotechnologies, with Dr. Hans-Hartmann Pedersen (EC Research Programme Officer) as EC Observer. This meeting in Brussels was attended by at least fifteen FP7 and H2020 project coordinators and other representatives from research institutions and SMEs. ESSC is one out of the 19 European Clusters managed/ observed by DG R&I - KET - Unit Advanced Materials & Nanotechnologies. The ESSC [1] will identify technical or non-technical challenges for (bio)chemical sensing and highlight opportunities resulting from nanotechnology, microsystems integration, advanced data evaluation, their systemic integration as well as manufacturing and commercialization based on an application and demand driven approach. ESSC will mobilize a pan-European network, ready to advise, assist and implement national and international measures to strengthen the position of European research and innovation. The ESSC key areas have been identified: Environmental Sustainability, Energy Efficiency, Health Monitoring, Comfort, Industrial Applications. [1] M. Penza et al., AMA Science, Open Access. DOI: 10.5162/4EuNetAir2015/08

10:00 *Coffee break*

Functional Materials for Energy and Monitoring Systems : Marcel Bouvet

10:30 Naked-eye readable zero power optical hydrogen sensor using biomimetic nano-actuator **X.XIII.1**

Authors : Heetak Han1, Sangyul Baik2, Jungmok Seo3, Changhyun Pang4, Taeyoon Lee1
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Resume : For the last few decades, there have been a great effort to use hydrogen (H2) as an alternative energy instead of fossil fuel due to its renewable, energy efficient and eco-friendly properties. However, intrinsic properties of H2 such as colorless, odorless and tasteless make people hesitate to use the explosive H2 in household or vehicle. Therefore, sensing technology for H2 becomes more important along with increasing demands of safe use of H2 and various sensing techniques has been developed such as

electrical, electrochemical, mechanical and optical types of devices. Among these technologies, optical based H2 sensors have attracted more attention from researchers due to its working principle which does not involve the use of electrical components in the sensing area. However, optical H2 sensors that have been developed to date have limitations in their performances such as a sensitivity, response and relaxation time due to intrinsic properties of sensing materials. In this research, we fabricated optical H2 sensors based on a nano-actuator inspired from sensing organs of insects. In order to implement the nano-actuator, first of all, micro/nano-pillar arrays of polyurethane were fabricated using simple molding process. Next, thin palladium (Pd) layer was obliquely deposited onto the only one side of each pillar. Then, the pillars were bent by the residual stress generated in the metal film and the bending angle of the pillars were immediately affected by the H2 concentration due to volume expansion of the Pd layer under H2 exposure. Since optical properties of nano-actuator were also dramatically changed by the change of the bending angles of nano-pillars, the nano-actuator was applied to highly sensitive optical H2 sensor. The biomimetic nano-actuator-based optical H2 sensor shows high sensitivity, fast response time and stable repeatability which are clearly recognizable the naked human eye.

10:45 Electrolyte effects in manganese oxides in context of water electrolysis : in situ Raman and corrosion studies **X.XIII.2**

Authors : Chinmoy Ranjan, Zoran Pavlovic , Qiang Gao, Raoul Blume, Robert Schloegl
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Resume : Non noble metal "earth abundant" electrocatalysts will significantly reduce the costs and make it possible to use electrochemical water splitting (electrolysis) on a very large scale. Non noble metal catalysts can be an effective replacement even if their electrochemical activities are a fraction of their noble metal counterparts. If these catalysts can be developed to an extent where their operational lifetime would become comparable to their noble metal counterparts, a large part of the problem would be solved. MnO2 is earth abundant and well known for catalyzing oxygen evolution. A form of MnOx cluster is known to catalyze water oxidation in photosynthesis. In order to understand the limitations of this catalyst under the operational conditions, it is important to study this material in situ. Electrodeposited of MnOx on the surface of Au was studied using in situ Surface Enhanced Raman Spectroscopy (SERS) is used for tracking the structural changes of hydrous MnOx. Besides in-situ study of catalyst structure, ex situ analysis of corrosion using flow cells combined with atomic emission spectroscopy was carried out alongside explicit detection of oxygen. Various kinds of electrolytes were used to evaluate the effects of cations, anions and solution pH on molecular structure and performance of MnOx catalysts. Charge to radius ratio of alkali metal ions affected the reactivity of the oxides and was seen to influence reaction under both potentiostatic and potentiodynamic conditions with Li+ and (K+, Cs+) containing electrolytes showing the lowest and highest activities respectively. Strong effects on catalyst structure and performance were also seen when various anions such as perchlorate or borate were inluded in the electroytes being investigated.

11:00 Integration of photosensitive valves for automated in-situ microfluidic control **X.XIII.3**

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Resume : Development of scalable systems for continuous, in-situ monitoring of water quality remains one of the main challengesforenvironmental research and sustainability. While extensive literature describing new sensing methods and innovative analytical approaches has been published overthe past twenty years, no practical solutionfor affordable integratedanalytical platforms has been proposed. Additionally, the high cost of fabrication of complex fluidic designs and components such as pumps and valves required for these platforms has further restricted the ability to produce an affordable option for end-users outside of government agencies and specialized commercial entities. The development of new materials and device concepts to replace these bulky and expensive components has the potential to generate breakthroughs in the development of cost-effective and reliable monitoring systems. In this paper, the impact of introducing new rapid prototyping techniques and innovative fabrication approaches to the optimization of biomimetic fluidic handling components, specifically light-responsive hydrogel valves fully integrated within microfluidics systems are presented.This provides a low-cost, low-energy and non-contact, scalableapproach to integration of these critical fluid handlingcomponents. The in-situ nature of the valves results in a significant elimination of dead volume in the system, due to the need to site conventional macro

valves off-chip. A fully automated prototype LED-triggered platform has been produced to demonstrate various cycles of opening and closing of the polymer-gel valves. This project has received funding from the European Unions Seventh Framework Programme for research, technological development and demonstration under grant agreement no. 604241 Scope:Materials /Hybrid materials: from the laboratory to the market

11:15 Hysteresis-Free Nanoplasmonic Pd-Au Alloy Hydrogen Sensors **X.XIII.4**

Authors : Ferry A. A. Nugroho*, Beniamino Iandolo**, Carl Wadell*, Emil Lidström*, Jakob B. Wagner**, Christoph Langhammer*
Affiliations : *Department of Physics, Chalmers University of Technology SE-412 96, Göteborg, Sweden; **Center for Electron Nanoscopy, Technical University of Denmark, 2800 Kongens Lyngby, Denmark.

Resume : The imminent prospect of a hydrogen economy and recent market introduction of hydrogen fuel cell cars demand a development of safe and reliable hydrogen sensors. Hydrogen sensors are also becoming increasingly important in many industrial processes, food industry and in health monitoring. Specifically for fuel cell cars, stringent performance targets have been set by the automotive industries to ensure a safe operation [1]. In this regards optical sensors are beneficial because they provide means for remote readout and are considered safer than electrical sensors as they pose no risk of spark generation. A growing avenue within the field of optical hydrogen sensors is the use nanostructured metal-hydride systems as signal transducer in plasmonic hydrogen sensors [2]. For this application, palladium (Pd) has been the main transducer material since it readily absorbs and releases hydrogen at RT. However, pure Pd exhibits wide hysteresis upon sorption which creates ambiguous readout depending on the sensor's history. To this end, alloying the hydride-forming metal with another metal (i.e. Pd−Au) has been known to reduce the hysteresis. In this work we present a novel plasmonic optical hydrogen sensor using Pd−Au alloy nanoparticles [3] and its generic fabrication strategy [4]. As the key features of our study, by increasing the Au content in the alloy nanoparticles up to 25 at.%, we find an eight-fold sensitivity increase in the sub-10 mbar pressure range (i.e. the critical pressure range before hydrogen reaches its flammability limit at 40 mbar) compared to a pure Pd, sensor accuracy < 5% throughout the studied 1 mbar−1 bar hydrogen pressure range and, by engineering the sensor nanoparticle size, sub-second sensor response times. Thus we meet or exceed the performance targets set by the automotive industry. Finally we also report a distinct wavelength-independence of the qualitative sensor response to hydrogen pressure. This opens up the possibility to use single-wavelength plasmonic hydrogen sensing, which promises the use of low-cost optical components such as cheap LED light sources and a simple photodiode detector for implementation in real devices. References (1) Boon-Brett, L.; Bousek, J.; Black, G.; Moretto, P.; Castello, P.; Hübert, T.; Banach, U. Identifying Performance Gaps in Hydrogen Safety Sensor Technology for Automotive and Stationary Applications. Int. J. Hydrogen Energy 2010, 35, 373–384. (2) Wadell, C.; Syrenova, S.; Langhammer, C. Plasmonic Hydrogen Sensing with Nanostructured Metal Hydrides. ACS Nano 2014, 8, 11925–11940. (3) Wadell, C.; Nugroho, F. A. A.; Lidström, E.; Iandolo, B.; Wagner, J. B.; Langhammer, C. Hysteresis-Free Nanoplasmonic Pd-Au Alloy Hydrogen Sensors. Nano Lett. 2015, 15, 3563–3570. (4) Nugroho, F. A. A.; Iandolo, B.; Wagner, J. B.; Langhammer, C. Bottom-Up Nanofabrication of Supported Noble Metal Alloy Nanoparticle Arrays for Plasmonics. Submitted. 2015.

11:30 Modified porous conductive materials as catalyst supports **X.XIII.5**

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Resume : In the last years many groups have focused their research on improving the transport properties of high surface area materials as ideal support for different applications, such as sensors, drug delivery or catalysis. The combination of high surface area with high electrical conductivity is still a challenge, since the chemical approaches to both features are mutually exclusive. In this work, we present a novel and versatile supporting porous material with significant electrical conductivity and high surface area. Our strategy consists of the combination of an insulating porous framework modified on the surface by a transparent conductor oxide to yield excellent surface conductivity, while maintaining the highly porous structure. As a proof of concept we have use this highly porous electrodes to support a coordination polymer of the Prussian blue (PB) family that promotes the water oxidation at neutral pH and ambient conditions. [1] Complete characterization of these electrodes using X-ray Diffraction (XRD)

Environmental Scanning Electron Microscopy (ESEM) and electrical characterization of the surface were carried out to determine the penetration and the interaction of the PB with the conductive surface. Correlations with their enhanced electrocatalytic features allowed maximizing current densities and stability.

11:45 CO2 Detection and Plasmonic Nanospectroscopy of CO2 Adsorption Energetics in Porous Sorbents for CCS **X.XIII.6**

Authors : Ferry A. A. Nugroho*, Chao Xu**, Sara Nilsson*, Michael Persson***, Niklas Hedin**, Christoph Langhammer*
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Resume : The Carbon Capture and Storage (CCS) scheme aims to reduce the amount of CO2 in the atmosphere. One main research direction in CCS is the development of new materials for CO2 capture and detection whose qualities are often assessed by measuring their isosteric heat of adsorption (Qst) using various methods based on gravimetric and volumetric measurement principles. These methods, however, often require precise determination of initial sample weight and/or volume. Therefore it is very appealing to develop an alternative method where such necessities are absent. In the past years, the optical indirect nanoplasmonic sensing (INPS) [1] platform has established itself as a powerful and versatile experimental tool to study functional materials at the nanoscale. Its merits include superior sensitivity down to individual nanoparticles [2], possibility for in situ and in operando experiments under a wide range of conditions, a relatively simple setup and flexibility in terms of the studied sample materials ranging from thin films to nanoparticles, as they can be conveniently deposited on top of the sensors. In this work we demonstrate how INPS can be an attractive alternative to detect and characterize the gas adsorption process in a micro- or mesoporous sorbent material. Specifically, we show how the CO2 isosteric heat of adsorption (Qst) of thin microporous PIM-1 polymer films and of amine-functionalized large-scale commercially available silica nanoparticles can be conveniently obtained without any calibration; as opposed to the conventional methods [3]. Thus, this study provides a generic blueprint for a plasmonic CO2 detection scheme and for efficient optical screening of micro- and mesoporous sorbent materials for CCS or other CO2/gas separation processes in terms of their adsorption energetics and kinetics. References (1) Langhammer, C.; Larsson, E. M.; Kasemo, B.; Zorić, I. Indirect Nanoplasmonic Sensing: Ultrasensitive Experimental Platform for Nanomaterials Science and Optical Nanocalorimetry. Nano Lett. 2010, 10, 3529–3538. (2) Syrenova, S.; Wadell, C.; Nugroho, F. A. A.; Gschneidtner, T. A.; Diaz Fernandez, Y. A.; Nalin, G.; Świtlik, D.; Westerlund, F.; Antosiewicz, T. J.; Zhdanov, V. P.; et al. Hydride Formation Thermodynamics and Hysteresis in Individual Pd Nanocrystals with Different Size and Shape. Nat. Mater. 2015, 14, 1236–1244. (3) Nugroho, F. A. A.; Xu, C.; Hedin, N.; Langhammer, C. UV-Vis and Plasmonic Nano-Spectroscopy of the CO2 Adsorption Energetics in Microporous Polymers. Anal. Chem. 2015, 87, 10161–10165.

12:00 Membranes for Hydrogen Purification and Enrichment of Impurities for Purity Analysis of Fuel Cell Hydrogen **X.XIII.7**

Authors : Ruth Hill-Pearce and Arul Murugan
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Resume : By 2030 we are to expect 1,100 hydrogen refuelling stations in operation in the UK [1], supplying high purity hydrogen to 1.6 million fuel cell vehicles. Despite this great surge in hydrogen technologies, fuel cell degradation, caused by impurities in hydrogen, remains a major issue [2]. The ISO 14687-2 standard specifies the maximum limits of 13 gaseous impurities ranging from 4 nmol mol-1 to 300 ï¿½mol mol-1 [2]. The consensus from analytical laboratories is that the measurements required for this qualitative assurance step are not currently possible at the stated amount fractions [3]. Additionally, the analysis of all impurities in the standard with commercially available techniques would be excessively time-consuming and prohibitively expensive. Pre-concentration of the impurities using an enrichment device enables lower cost measurements and reduces analysis time and the need for expensive state-of-the-art analysers. The enrichment device uses membranes which are selectively permeable to protons, we investigate the suitability of membranes for this device and for hydrogen purification providing confidence in these membranes after prolonged use. Using dense Pd/Au membranes in the enrichment device we have shown that some reactive species such as carbon monoxide, methane and hydrogen sulphide react in the enrichment chamber or adsorb

on the membrane wall during enrichment [4]. This loss or gain in impurities during the enrichment process leads to deviation from the calculation of the enrichment factor. A gas testing rig has been built at NPL to enable membranes to be subjected to controlled gaseous environments through use of our suite of primary gas reference standards, enabling the accurate quantification of the loss or gain in amount fraction of the key reactive impurities in hydrogen during the enrichment process. We investigate the chemical reactions occurring and the loss of species due to adsorption on the membrane walls using downstream gas impurity analysis and surface analysis techniques including XPS and SIMS. The possibility of quantifying the adsorbed impurities using these techniques during the regeneration or cleaning of the membranes by temperature programmed desorption is also investigated. 1. UK H2 Mobility, Phase 1 Results. In https://www.gov.uk/government/uploads/system/uploads/attachment_data/file/192440/13-799-uk-h2-mobility-phase-1-results.pdf, 2013. 2. ISO 14687-2. In http://www.iso.org/iso/home/store/catalogue_tc/catalogue_detail.htm?csnumber=55083, 2012. 3. Murugan, A.; Brown, A. S. International Journal of Hydrogen Energy 2015, 40, (11), 4219-4233. 4. Murugan, A.; Brown, A. S. Analytical Methods 2014.

Closing remarks : Michele Penza

12:30 Closing remarks **X.XIII.8**

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Resume : Closing remarks

12:45 *Lunch*

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