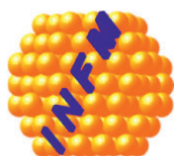


# INTERNATIONAL WORKSHOP OF MATERIALS PHYSICS

## PROGRAM and ABSTRACT BOOK



**4<sup>th</sup> edition of  
International Workshop of Materials Physics**

**28<sup>th</sup> -29<sup>th</sup> of May 2019**

**Invited Lectures**



FUNDAȚIA "CULTURĂ ȘI FIZICĂ LA MĂGURELE"



**4<sup>th</sup> edition of the  
INTERNATIONAL WORKSHOP OF MATERIALS PHYSICS**

**28<sup>th</sup>-29<sup>th</sup> May 2019**

The National Institute of Materials Physics (NIMP) announces the organization of the 4<sup>th</sup> edition of the International Workshop of Materials Physics (IWMP). The topic for 2019 edition is dedicated to energy, with special focus on topics such as: photovoltaics (novel photo-effects, halide perovskites, new architectures for solar cells, etc.), energy harvesting (piezo, pyro, thermoelectric), fusion, energy storage, energy transport, and other similar topics. Aspects related to modeling, fabrication, characterization will be presented and discussed.

Similar to the first three editions, the 4<sup>th</sup> edition of IWMP is organized on invitation only. The aim is to attract well known researchers in the field, the final purpose being to establish new collaborations concretized in common publications, projects and exchange of personnel.

Young researchers willing to present their latest results on topics related to the main topic of the workshop are invited to submit a 2 page abstract (A4, Times New Roman 11, single spacing, 2 cm margins, including figures and references) to the organizers ([pintilie@infim.ro](mailto:pintilie@infim.ro)). The best abstracts will be selected for oral presentations during the workshop.

The workshop will take place at NIMP premises located in Magurele, Romania.

The topics for the next two editions:

2020-Materials and structures for bio-applications

2021-Recent developments in the field of ferroelectrics and multiferroics

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## Program

29<sup>th</sup> of May

2019

8:15-8:50

REGISTRATION

8:50-9:00

OPENING

9:00-11:15

Session 1

9:00-9:30

Magdalena Titirici

Department of Chemical Engineering, Imperial College London,

**Going green with black: On Biomass, Carbon and Clean Energy**

9:30-10:00

Vladimir Matolin

Charles University, Czech Republic

**PEM Based Ordered Superstructures as a Durable  
Support for Fuel Cell Catalyst**

10:00-10:30

Ifan Stephens

Imperial College London, UK

**Power-to-X: the role of catalysis in advancing the electrochemical  
synthesis of our most coveted chemicals**

10:30-11:15

Mihaela Florea

**Cost efficient oxygen generation through alkaline  
water electrolysis using Ni on SnO<sub>2</sub> mesoporous support-based electrocatalysts**

Adela Nicolaev

**Carbon monoxide adsorption, dissociation and oxidation on ferroelectric  
surfaces decorated with nanoparticles of noble metals**

Stefan Neatu

**The use of three-component composites in the  
photocatalytic water splitting reaction**

11:15-11:30

COFFEE BREAK

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11:30-13:00

Session 2

11:30-12:00

Joe Briscoe

Queen Mary University London, UK

**Sustainable energy devices using nanostructured polar materials**

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12:00-12:30

Andrew Holmes

Imperial College London, UK

**Piezoelectric Devices for Energy Harvesting from Motion and Flow**

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12:30-13:00

Sam Cooper

Imperial College London, UK

**Multilength scale characterisation of materials, microstructures and performance of batteries and fuel cells.**

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13:00-14:30

**LUNCH**

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14:30-16:30

Session 3

14:30-15:00

Marin Alexe

University of Warwick, UK

**Bulk- and Flexo-Photovoltaic effects**

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15:00-15:30

George A. Nemnes

**Measurement protocols for a reliable electrical characterization of perovskite solar cells**

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15:30-16:00

Anca Duta

Transilvania University Brasov

**VIS-active photocatalytic composites for advanced wastewater treatment**

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16:00-16:30

Lucia Leonat

**Reticulated mesoporous TiO<sub>2</sub> scaffold for hybrid perovskite solar cells**

Mihai Grigoroscuta

**Improved performance of a Si-solar cell by up- conversion in Yb/Er doped CeO<sub>2</sub> thin films**

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16:30-18:00

**VISIT TO NIMP FACILITIES**

18:00

**DEPARTURE FOR DINNER**

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29<sup>th</sup> of May 2019

9:00-11:15

Session 4

9:00-9:30

Andrei.V. Kovalevsky

CICECO – Aveiro Institute of Materials,

Department of Materials and Ceramic Engineering, University of Aveiro, Portugal

**Selected approaches for designing oxide thermoelectrics**

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9:30-10:00

Andres Sotelo

ICMA-CSIC-Universidad de Zaragoza, Spain

**Very high thermoelectric performances in Sr-doped textured  $\text{Ca}_3\text{Co}_4\text{O}_9$ .**

**Costs optimization of unileg thermoelectric generator fabrication.**

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10:00-10:30

Ernst Bauer

Technische Universität Wien, Austria

**Bulk and thin film Heusler alloys as promising thermoelectric materials**

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10:30-11:15

Bogdan Popescu

**Thermoelectric nano-composite from double filled  
skutterudite and carbides**

Ionel Mercioniu

**On the adherence of ceramic layers for thermal barriers coatings**

Magdalena Galatanu

**Development of thermal barriers materials with application in energy**

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11:15-11:30

**COFFEE BREAK**

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11:30-13:15

Session 5

11:30-12:00

Mihai A. Gîrțu

Department of Physics and Electronics,

Ovidius University of Constanța, Constanța, Romania

**DFT Calculations of Structure and Electronic Properties of  
 $\text{TiO}_2$  Nanoclusters, of Dye-Nanocluster and Dye-Electrolyte  
Systems for Modeling Hybrid Photovoltaic and  
Photocatalytic Applications**

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12:00-12:30

Chris Chikere

School of Pharmacy and Life Sciences,  
Robert Gordon University, Aberdeen, UK

**New Electrode Materials for Energy Storage Devices-Battery Applications**

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12:30-13:15

Oana Rasoga

**Tryphenylamine and carbazol oligomers for photovoltaic applications**

Silviu Polosan

**Organometallic compounds for photovoltaic applications**

Mihaela Baibarac

**Composites based on carbon nanotubes and polydiphenylamine: from the functionalization process to applications in the energy storage field**

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13:15-14:45

**LUNCH**

14:45-17:00

**Session 6**

14:45-15:15

Ibrahim Burc Misirlioglu

Sabanci University Istanbul, Turkey

**Functionality from ferroelectric superlattices:**

**Designing a phase transition and its implications for applications**

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15:15-15:45

Andrei Manolescu

University of Reykjavik, Iceland

**Excitons in core-shell nanowires with polygonal cross section**

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15:45-16:15

Laura Abramiuc

**Photoelectron spectromicroscopy: revealing the stability of ferroelectric surfaces with respect to irradiation and contamination**

Adrian Crisan

**Nanotechnology of Pinning Centres in Superconducting Films for Clean Energy-saving Power Applications**

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16:15-16:30

**CLOSING**

16:45

**Departure for some sightseeing and dinner**

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## Bulk- and Flexo-Photovoltaic effects

Marin Alexe

University of Warwick, Department of Physics, CV4 7AL Coventry, UK

Two years after the invention of modern prototype solar cells, it was found that BaTiO<sub>3</sub> exhibits a photovoltaic effect distinct from that of p-n junctions, later called the bulk photovoltaic (BPV) effect. Under uniform illumination, a homogeneous ferroelectric material gives rise to a short-circuit current and produces an anomalously large photo-voltage well exceeding the bandgap energy. The microscopic origins of this effect supposed to originate from the asymmetric distribution of photoexcited non-equilibrium carriers in k-space, caused by absence of centrosymmetry.

The present talk will present a short history and the basics of the bulk photovoltaic effect, tip enhancement, as well as the electronic origin of the anomalous BPV in some materials such as BiFeO<sub>3</sub>. Later, potential applications such as energy harvesting or light-induced reversible switching of ferroelectric polarization at room temperature. I will show how the tip-enhanced effect may be used in optical switching tunnel junctions or other similar devices. Finally, we will discuss a new photovoltaic effect which turns the BPV effect into a universal effect allowed in all semiconductors by mediation of the flexoelectric effect. [1]

[1] M.-M. Yang D. J. Kim, & M. Alexe, Flexo-Photovoltaic Effect, Science 360, 904 (2018)

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## Bulk and thin film Heusler alloys as promising thermoelectric materials

B. Hinterleitner<sup>1,2</sup>, M. Poner<sup>1,2</sup>, Ch. Eisenmenger<sup>1</sup>, M. Stöger-Pollach<sup>1,3</sup>, Y. Kakefuda<sup>4</sup>,  
N. Kawamoto<sup>4</sup>, Q. Guo<sup>4</sup>, T. Baba<sup>4</sup>, T. Mori<sup>4,5</sup>, Yongpeng Shi<sup>6</sup>, Sami Ullah<sup>6</sup>,  
Qing Xie<sup>6</sup>, Xing-Qiu Chen<sup>6</sup>, and **E. Bauer**<sup>1,2</sup>

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<sup>2</sup>Christian Doppler Laboratory for Thermoelectricity, Technische Universität Wien, A-1040 Wien, Austria

<sup>3</sup>University Service Centre for Transmission Electron Microscopy,  
Technische Universität Wien, 1040 Wien, Austria

<sup>4</sup>National Institute for Materials Science (NIMS), International Center for Materials  
Nanoarchitectonics (WPI-MANA) and Center for Functional Sensor & Actuator (CFSN), Namiki 1-1,  
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<sup>5</sup>University of Tsukuba, Tsukuba 305-8671, Japan

<sup>6</sup>Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy  
of Science, School of Materials Science and Engineering, University of Science and Technology of  
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The energy transformation from one into another form (e.g. from a primary energy into electricity) and energy consumption are unavoidably associated with sizable losses, most of which occur in the form of heat. Recovering any fraction of this otherwise wasted heat would enhance the overall energy efficiency and thus contribute to counteract the energy crisis. Thermoelectric materials are able to convert temperature gradients into electricity and are thus ideally suited for this purpose. The energy conversion in a thermoelectric generator is based on a pure solid-state effect, the drift of charge carriers in a temperature gradient. As such, it is highly reliable, silent, maintenance free, and environment friendly. Presently, however, very few materials with sufficient performance, benchmarked by the so called figure of merit,  $ZT = S^2/(\rho\lambda)$ , are available on market.  $T$  is the absolute temperature,  $S$  the Seebeck coefficient,  $\rho$  is the electrical resistivity, and  $\lambda$  the total thermal conductivity, which is typically built by charge carriers and phonons, i.e.,  $\lambda = \lambda_e + \lambda_{ph}$ .  $\lambda_e$  is related to  $\sigma$  by the Wiedemann-Franz law.  $ZT$  values of at least 1 are required for a reasonably good performance of a TE device. Besides classical  $\text{Bi}_2\text{Te}_3$  related systems, only filled skutterudites are already produced on an industrial scale, as co-developed by authors of this abstract.

Heusler (1-2-1) and half-Heusler (1-1-1) alloys have been shown to provide a promising base for well performing thermoelectric materials and yield a rather robust characteristics for applications as thermoelectric generators. While the figure of merit  $ZT$  of half-Heusler alloys reached already values well above one, the overall performance of full Heusler alloys is still lacking such values.



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Although full Heusler systems are known for their large power factor, large thermal conductivities allow only moderate ZT values. To overcome such large thermal conductivities, we have prepared  $\text{Fe}_2\text{VAl}$  based alloys as thin films by magnetron sputtering. Subsequent studies on these systems revealed an unprecedentedly large value of the thermoelectric power factor  $pf$ . Since thermal conductivity is further suppressed for the films in comparison to the bulk material, the figure of merit, ZT, is larger than values reported in literature. Various observations have been made, supposed to be responsible for the superior performance of thin films based on  $\text{Fe}_2\text{VAl}$ . Among others, there are i) a meta-stable state which causes a change from fcc to bcc; ii) an electronic density of states exhibiting huge logarithmic energy derivatives, iii) Weyl nodes close to the Fermi energy, and iv) an arrangement of atoms in the crystalline unit cell, reminiscent of high entropy alloys with random disorder on all lattice sites.

Research supported by the “Christian Doppler Laboratory for Thermoelectricity” and by JST under the program CREST.

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# Sustainable energy devices using nanostructured polar materials

**Joe Briscoe**

Queen Mary University London, UK

A theme that runs through much of my group's research is the use of nanostructured polar materials, such as piezoelectrics and ferroelectrics, to produce or enhance energy conversion from sustainable sources, such as solar and kinetic (movement and vibrations). This talk will give a tour of some of the key examples of this work, as well as giving a preview of some of the complementary work that we do in novel processing techniques for photovoltaic (PV) materials.

First, an overview of our research into nanostructured piezoelectric energy harvesters using ZnO nanorods (nanogenerators) will be presented. Examples of our past and present research into ferroelectrics for photocatalysis and photoelectrocatalysis will then be given, and finally a preview of our recent developments in using aerosol-assisted chemical-vapour deposition (AACVD) to produce hybrid lead halide perovskite PVs.

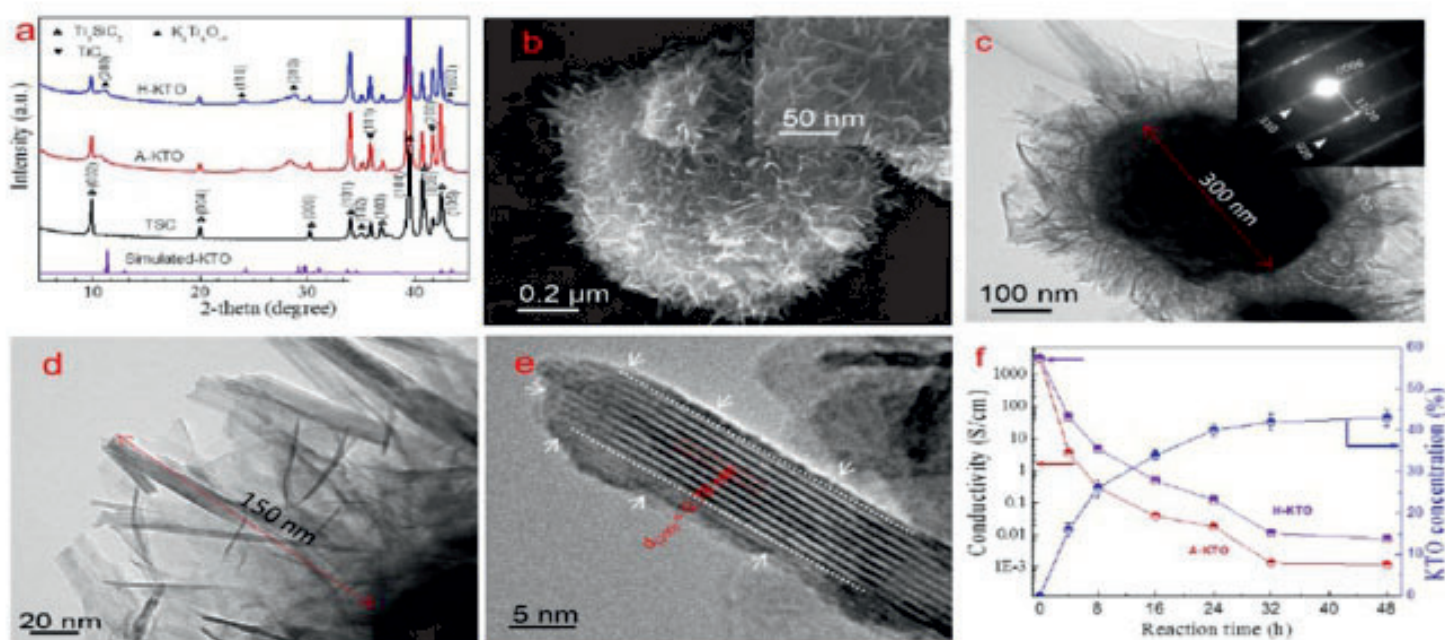
# New Electrode Materials for Energy Storage Devices- Battery Applications

C. Fernandez<sup>1</sup> and C. Chikere<sup>1</sup>

1. School of Pharmacy and Life Sciences, Robert Gordon University, Aberdeen, United Kingdom  
c.o.chikere@rgu.ac.uk and c.fernandez@rgu.ac.uk

Our research interest has been focused on two main areas of Physical Chemistry which includes energy storage devices (batteries) and electrochemical sensors. We lay emphases on the synthesis and utilization of new materials for battery applications (energy storage devices). 2D materials such as graphene, carbides, nitrides, oxides, and chalcogenides have recently attracted broad interest because of their unique structural and chemical properties, which make them promising electrode materials for new-generation Lithium-ion batteries (LIBs). Among these 2D materials, the group of transition-metal carbides labelled as MXene ( $\text{Ti}_3\text{C}_2(\text{OH}_x\text{F}_{1-x})_2$ ), are potential electrode materials for LIBs because of their layered structure similar to that of graphite, providing effective lithium storage space.

A new class of core-shell MAX@K<sub>2</sub>Ti<sub>8</sub>O<sub>17</sub> by alkalization hydrothermal reaction and hydrogenating, which bestows high sodium ion intercalation pseudo-capacitance for sodium-ion batteries applications. The distorted dodecahedrons between layers not only provide abundant sites of sodium-ion accommodation but also act as wide tunnels for sodium-ion transport.



**Figure 1.** Material characterisation a) XRD patterns of different samples b) A representative FESEM image of H-KTO composite. The inset shows a high magnification of local image. c) Typical TEM image of core shell H-KTO sample. The inset corresponds to the AED image of exterior shell layer (K<sub>2</sub>Ti<sub>8</sub>O<sub>17</sub>). d) A high magnification of exterior shell layer (K<sub>2</sub>Ti<sub>8</sub>O<sub>17</sub>). e) HRTEM image of the (K<sub>2</sub>Ti<sub>8</sub>O<sub>17</sub>) plate. f) Effect of reaction time on conductivity and KTO concentration of different samples.

The synthesis of MXene/Ag composite have been demonstrated. The compound can be deemed as an excellent anode material for lithium-ion batteries, exhibiting an extraordinary long cycle lifetime with a large capacity at high charge–discharge rates. Remarkably, the composite withstands more than 5000 cycles without capacity decay at 1–50 °C.

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The main reasons that the long cycle life with high capacity are relevant to the reduced interface resistance are due to the occurrence of Ti (II) to Ti (III) during the cycle process.

Zinc oxide nanoparticles (nano-ZnO) was used to modify carbon paste electrode (CPE) for a fast and sensitive electrochemical determination of gallic acid (GA). The study was carried out using cyclic voltammetry (CV) and differential voltammetry (DPV) techniques, where the nano-ZnO-modified electrode exhibited an efficient and sensitive oxidation of GA. The cyclic voltammetric result showed a significant enhancement of the peak current from 250 A to about 410 A. The electrochemical behaviour of GA on the nano-ZnO modified carbon paste electrode was studied using DPV, showing a sensitivity of the electrode in a concentration range of  $1 \times 10^{-6}$  to  $5.0 \times 10^{-5}$  mol L<sup>-1</sup>, with a correlation coefficient R<sup>2</sup> of 0.9968 and a limit of detection of  $1.86 \times 10^{-7}$  mol L<sup>-1</sup> (S/N =3). The proposed electrode was used successfully for the determination of GA in red wine with recoveries of 103%.

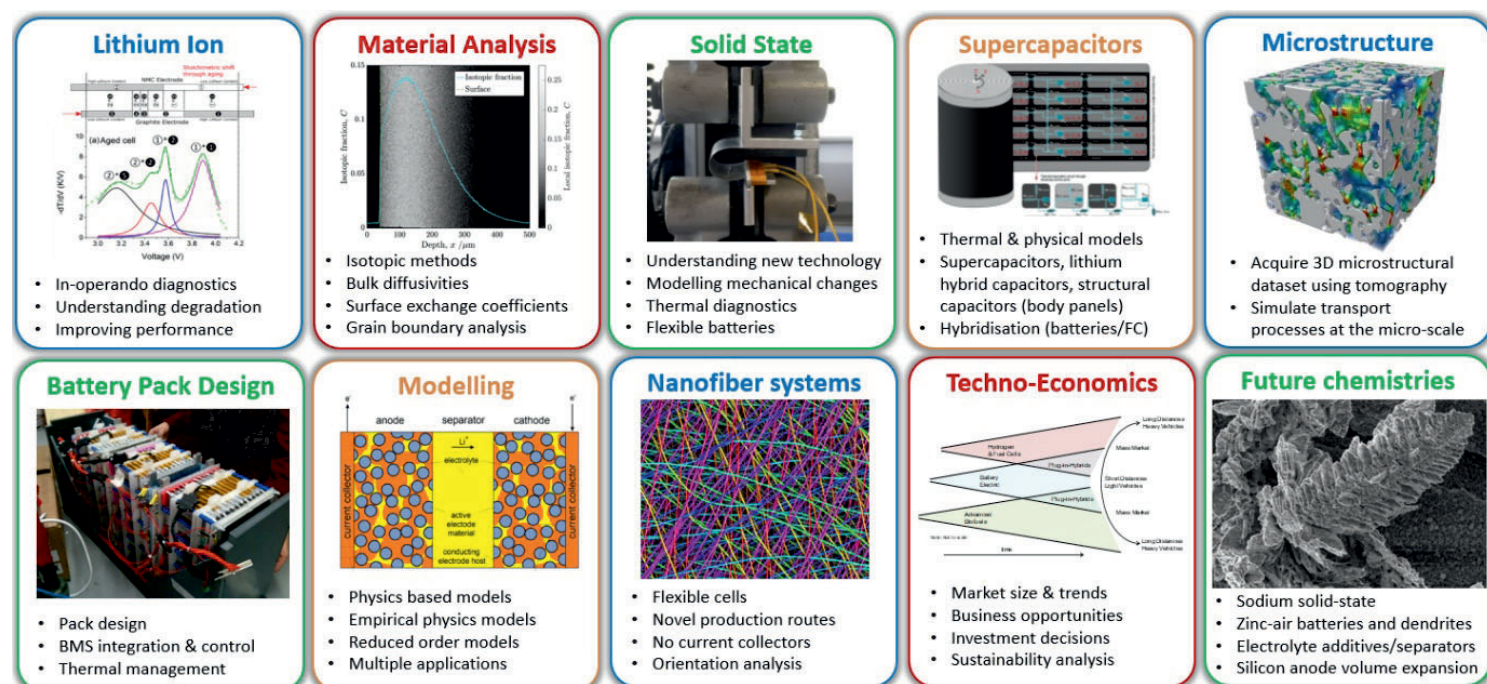
Zirconium oxide nanorods (ZrO<sub>2</sub>) have been used for the first time in the modification of a carbon paste electrode (CPE) for the determination of gallic acid (GA). The voltammetric results of the ZrO<sub>2</sub>-modified CPE showed an efficient electrochemical oxidation of gallic acid, with a significantly enhanced peak current from  $260.9 \text{ A} \pm 3.2$  to about  $450.8 \text{ A} \pm 1.09$ . Meanwhile the electrochemical behaviour of GA on the surface of the modified electrode was studied using differential pulse voltammetry (DPV), showing a sensitivity of the electrode for GA within a concentration range of  $1 \times 10^{-6}$  mol L<sup>-1</sup> to  $1 \times 10^{-4}$  mol L<sup>-1</sup> with a correlation coefficient of R<sup>2</sup> of 0.9945 and a limit of detection of  $1.24 \times 10^{-7}$  mol L<sup>-1</sup> (S/N = 3).

# Multilength scale characterisation of materials, microstructures and performance of batteries and fuel cells

**Sam Cooper**

Imperial College London, UK

This talk will highlight the work of the Electrochemical Science and Engineering group at Imperial College London, focusing in particular on some frequently encountered challenges and sources of uncertainty. The group consists of seven academics divided between three engineering departments and investigates electrochemical energy storage devices across a wide range of length and time scales, a selection of which are shown in the figure below.



Three-dimensional imaging forms a cornerstone of the ESE group's work, enabling the characterisation and analysis of microstructural data for battery, fuel cell and supercapacitor electrodes and separators. However, even the extraction of apparently conventional metrics, such as volume fractions and surface areas [1], present significant challenges in terms of the uncertainty inherent to the imaging and segmentation methods used. More advanced analysis approaches, including the simulation of the impedance responses of transport mechanisms [2], have been developed within the group and give rise to further questions about the validity of equivalent circuit based descriptions of device level data.

As part of the Faraday Challenge, the UK's major battery research initiative, we have designed a new family of isotopic exchange experiments, which enable the measurement of bulk diffusivities and surface exchange coefficients important for better understanding the performance of battery (and fuel cell) electrode materials [3]. However, once again, the workflow from preparation of consistent samples, through the exchange experiment itself and on to the secondary ion mass spectrometry analysis leads to significant uncertainty and difficulty of interpretation.



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Finally, at the device level, differential thermal voltammetry [4], amongst other more conventional battery characterisation methods, is being used to analyse the state-of-health of used cells, as well as to aid high dimensional cell sorting to maximise the value of second life packs. Transitioning this technique for a controlled lab environment to a high through-put industrial tool requires re-assessing what level of accuracy is truly necessary in the data in order to achieve the necessary performance.

- [1] S. J. Cooper, A. Bertei, P. R. Shearing, J. A. Kilner, and N. P. Brandon, “TauFactor: An open-source application for calculating tortuosity factors from tomographic data,” *SoftwareX*, vol. 5, pp. 203–210, 2016.
- [2] S. J. Cooper, A. Bertei, D. P. Finegan, and N. P. Brandon, “Simulated impedance of diffusion in porous media,” *Electrochim. Acta*, vol. 251, pp. 681–689, 2017.
- [3] S. J. Cooper, M. Niania, F. Hoffmann, and J. A. Kilner, “Back-exchange: a novel approach to quantifying oxygen diffusion and surface exchange in ambient atmospheres,” *Phys. Chem. Chem. Phys.*, vol. 19, no. 19, pp. 12199–12205, May 2017.
- [4] Y. Merla, B. Wu, V. Yufit, N. P. Brandon, R. F. Martinez-Botas, and G. J. Offer, “Novel application of differential thermal voltammetry as an in-depth state-of-health diagnosis method for lithium-ion batteries,” *J. Power Sources*, vol. 307, pp. 308–319, Mar. 2016.

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## VIS-active photocatalytic composites for advanced wastewater treatment

Tismanar I., Bogatu C., Covei M. , **Duta A.**  
Transilvania University of Brasov, Romania

Heterogeneous photocatalysis represents the current path investigated for advanced wastewater treatment, for the removal of organic pollutants at very low concentrations.

The reference photocatalyst is  $\text{TiO}_2$  that is efficient, aqueously stable and non-toxic. However,  $\text{TiO}_2$  is a wide band gap semiconductor thus it can only be activated using UV radiation and this represents one major barrier in the wider implementation of the photocatalytic processes. This is why various solutions were adopted to get VIS-active photocatalysts while preserving the already mentioned advantages.

One such solution is represented by the composite photocatalysts of  $\text{TiO}_2$  (an “n” type semiconductor) and a “p” type semiconductor, mimicking a photovoltaic cell. The  $\text{Cu}_2\text{ZnSnS}_4$  (CZTS) /  $\text{TiO}_2$  composite was layer by layer deposited on a FTO-coated glass substrate using Spray Pyrolysis Deposition (SPD) and proved to be more efficient in the photodegradation of the reference pollutant methylene blue, 20 ppm.

Following the same idea, CZTS was replaced by graphene oxide (GO) that is more aqueously stable as compared to CZTS. The composite layer was prepared by depositing a first  $\text{TiO}_2$  thin film by SPD that is afterwards annealed and a second layer of  $\text{TiO}_2$ -GO, obtained through sol-gel synthesis. To prevent the GO decomposition, annealing is not employed for this second layer and the deposition temperature is kept below  $180^\circ\text{C}$ .

This  $\text{TiO}_2$  - GO composite layer proved to be VIS-active and showed a very good aqueous stability and photocatalytic efficiency in the removal of MB 20ppm.

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# DFT Calculations of Structure and Electronic Properties of TiO<sub>2</sub> Nanoclusters, of Dye-Nanocluster and Dye-Electrolyte Systems for Modeling Hybrid Photovoltaic and Photocatalytic Applications

Corneliu I. Oprea,<sup>1</sup> Petre Panait,<sup>1,2</sup> Atoumane Ndiaye,<sup>1,3</sup> Anamaria Trandafir,<sup>1,4</sup>

Reda M. AbdelAal,<sup>5</sup> Fanica Cimpoesu,<sup>6</sup> **Mihai A. Gîrțu**<sup>1\*</sup>

<sup>1</sup>Department of Physics and Electronics, Ovidius University of Constanța, Constanța, Romania

<sup>2</sup>Faculty of Physics, University of Bucharest, Bucharest, Romania

<sup>3</sup>Department of Physics, Cheikh Anta Diop University of Dakar, Dakar, Senegal

<sup>4</sup>Department of Physics, University of Bath, Bath, United Kingdom

<sup>5</sup>Department of Chemical Engineering, Suez University, Suez, Egypt

<sup>6</sup>Department of Theoretical Chemistry, Institute for Physical Chemistry, Bucharest, Romania

\*E-mail: mihai.girtu@univ-ovidius.ro

We report results of a computational study of TiO<sub>2</sub> nanoclusters of various sizes as well as of complex systems with various molecules adsorbed onto the clusters, to set the ground for the modelling of charge transfer processes in hybrid organic-inorganic photovoltaics or photocatalytic degradation of pollutants. Despite the large number of existing computational studies of TiO<sub>2</sub> clusters and in spite of the higher computing power of the typical available hardware, allowing calculations of larger systems, there are still studies that use cluster sizes that are not appropriate to address particular problems or certain complex systems. By means of DFT calculations, we attempt to find acceptable minimal sizes of the Ti<sub>n</sub>O<sub>2n+2</sub>H<sub>4</sub> (n=14, 24, 34, 44, 54) nanoclusters in correlation with the size of the adsorbed molecule and the rigidity of the backbone of the molecule. Our calculations suggest that the n = 14 is a poor choice for simulating the materials used in the practical applications envisaged here. As the n = 24 cluster has provided mixed results, we argue that cluster sizes larger than or equal to n = 34 are necessary to provide the reliability required by photovoltaic and photocatalytic applications. Furthermore, the tendency to saturation of the key quantities of interest when moving from n = 44 to n = 54, suggests that the largest cluster may bring little improvement, at a significantly higher computational cost.

Additionally, we report results of DFT calculations to understand the dye regeneration mechanism of organic dyes in conjunction with cobalt(II) complexes. We are able to determine the parameters of Marcus' theory for electron transfer by means of density functional theory calculations of the energy in various dye-electrolyte configurations.



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# Piezoelectric Devices for Energy Harvesting from Motion and Flow

**Andrew S Holmes**

Professor of Microelectromechanical Systems  
Department of Electrical & Electronic Engineering  
Imperial College London

Over the past fifteen years, within the Department of Electrical and Electronic Engineering at Imperial College London, we have built up a significant research activity in micropower generation by energy harvesting, focusing mainly on motion-driven and flow-driven devices. This work has covered generalised analysis of micropower generator architectures, detailed design, fabrication and testing of microgenerator devices and work on power processing in energy harvesting systems. This talk will open with a broad overview of these activities. It will then take a more detailed look at two particular devices we have worked on in recent years. The first is a piezoelectric energy harvester for human body motion which employs frequency up-conversion via magnetically coupled plucking of a piezoelectric beam. The second is an airflow-driven energy harvester based on the galloping instability exhibited by a piezoelectric cantilever with a bluff body attached to its free end. This device shows an approximately linear variation in vibration frequency with flow velocity, making it potentially useful as a self-powered wind-speed sensor.

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## **Selected approaches for designing oxide thermoelectrics**

**A.V. Kovalevsky**

CICECO – Aveiro Institute of Materials, Department of Materials and Ceramic Engineering,  
University of Aveiro, 3810-193 Aveiro, Portugal

Thermoelectric (TE) effect provides an elegant solution for conversion of the waste heat into electrical energy, based on the intrinsically simple technology employing no moving parts and possessing self-sufficiency to enable mobile or remote applications. In some energy-conversion scenarios the cost and thermal stability requirements may dominate over efficiency issues, making abundant, high-temperature-stable and low-toxic oxides an interesting alternative TE material. The talk will focus on opportunities for high-temperature thermoelectric energy harvesting and feature some promising strategies to design performing oxide-based thermoelectrics. Particular attention will be given to the approaches where inherent redox flexibility of oxides is invoked for tailoring the functional TE properties, and some nanocomposite concepts.

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# Electricity saving with gallium oxide power electronics; perspectives, challenges and our focus on understanding and controlling defects in this material

**Andrej Kuznetsov**

Department of Physics and Centre for Material science and Nanotechnology,  
University of Oslo, Pb 1048 Blindern, 0316 Oslo, Norway

The physics of gallium oxide ( $\text{Ga}_2\text{O}_3$ ) – an interesting wide bandgap semiconductor – is currently under intensive investigations within a broad research community. This interest is because of the exceptional fundamental properties of  $\text{Ga}_2\text{O}_3$  very promising for power electronics, and of potential use in a range of other applications, e.g. in solar blind photodetectors, scintillators for medical diagnostics, transparent and passivating layers in solar cells, detectors tolerating high radiation/temperature, etc. As such, the potential technological impacts are manifold; to name just one – for power electronics – changing from the presently dominating Si (or even more advanced SiC) to  $\text{Ga}_2\text{O}_3$ , will save tremendous amount of electricity otherwise lost in operation. Indeed, according to a recent “Wide Bandgap Power Electronics Technology Assessment” by the US DoE over 25% of the worldwide annual energy consumption can be saved if widespread (>90%) adoption of the wide band gap power electronics technologies can be realized. For power electronics, among other materials,  $\text{Ga}_2\text{O}_3$  possess most superior properties (humbled by diamond only), as such ranking it increasingly high among other “energy” materials.

One of the issues slowing down the use of  $\text{Ga}_2\text{O}_3$  is the lack of fundamental understanding and difficulties in controlling electrically active point defects and defect complexes. Indeed, starting from “simplest” point defects, due to the low symmetry of typically used monoclinic  $\beta\text{-Ga}_2\text{O}_3$ , there are two different configurations of Ga in the unit cell (tetragonal and octagonal, GaT and GaO, respectively) and three different environments in the O sub-lattice in  $\beta\text{-Ga}_2\text{O}_3$ . Such complexity results in equally many different vacancy configurations and sites for extrinsic impurities to reside, provoking a number of electronic states in the bandgap. Further, taking into consideration potential extrinsic impurities and corresponding defect complexes, the result is a plethora of potential localized electronic states.<sup>1</sup> Some initial understanding has been accounted recently, not least with an active participation of our team.

In this presentation, upon discussing the perspectives and challenges for the use of gallium oxide in power electronics, the results of our recent investigations<sup>2</sup> of electrically active levels in  $\beta\text{-Ga}_2\text{O}_3$  will be highlighted and set in the context of the present understanding. Our strength is in using a combination of the deep level transient spectroscopy (DLTS), secondary ion mass spectrometry (SIMS), proton irradiation for controllable introduction of the intrinsic defects, and hybrid functional calculations for guiding the experimental work. Among other data, rather unique observations of thermally activated defect reconstructions stimulated by applied electric field will be shown and discussed, as such broadening the impact of the data beyond a specific methodology in a specific material.

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## Excitons in core-shell nanowires with polygonal cross section

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We describe the formation of excitons in a tubular prismatic geometry representing the outer layer of a core-shell nanowire. We use a numerical approach based on a multi-electron Hamiltonian, with valence and conduction bands, which includes the Coulomb interaction. We focus on the implications of the quantum localization in the corners or on the sides of the polygonal cross section. We compare the results of the multi-electron method with those of an electron-hole model and we show that the latter does not reproduce all exciton energies.

Our models explain recent experimental photoluminescence spectra obtained on asymmetric hexagonal shells.

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## PEM Based Ordered Superstructures as a Durable Support for Fuel Cell Catalyst.

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Nowadays fuel cell technology is accounted as a viable source of clean energy meeting requirements of carbon-free economy. However, high cost of the technology and limited level of durability are still obstacles on the way of successful commercialization. State of the art fuel cell catalyst layer is based on carbon supported Pt or Pt-based nanoparticles mixed with an ionomer. Despite the acceptable levels of performance this catalyst layer has thickness up to 10  $\mu\text{m}$ , which imposes certain limitation of the reactants/products transport and reduces utilization of the catalyst. Moreover, relatively stable, at working fuel cell potentials, carbon support shows significant degradation at potentials higher than 1.2 V, which limits overall stability of the fuel cell.

On the other hand, employment of the carbon-free ordered nanosupports has already shown a promising stability and high levels of the Pt utilization. In our work we have shown novel approach of preparation of such supports using the etching/deposition treatment of Nafion membrane during magnetron sputtering of  $\text{CeO}_2$ . Treatment of membrane develops deep vertical pores and ionomer nanopillars without a noticeable decrease of membrane thickness. The magnetron sputtering of Pt on these nanostructures leads to the formation of fine nanoclusters with size of about 5 nm. Resulting structures have demonstrated high levels of performance on both sides of the fuel cell. This structure demonstrates high level catalyst utilization on the cathode side reaching up the level of 15  $\text{kW/g}_{\text{Pt}}$ .

Membrane electrode assemblies (MEAs) with 20  $\mu\text{g}/\text{cm}^2$  on anode and commercial cathode and the all-commercial catalyst assembly exhibit the same level of performance. Accelerated stress test (AST) cycling between potentials 1 – 1.5 V causes only limited degradation with 15 % loss of the initial electrochemical active surface area (ECSA) for the proposed structure, which contrasts to the almost 90% loss for commercial catalyst assembly. At last it worth stress that method proposed in our study allows to prepare efficient catalysts in two steps, which improves reproducibility and decreases cost of the catalyst preparation.

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# Functionality from ferroelectric superlattices: Designing a phase transition and its implications for applications

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Ferroelectric-paraelectric phase transitions in thin films have occupied the agenda of numerous groups since late 1980s with the emergence of the possibility to grow ferroelectric thin films on misfitting substrates. Sometimes also called “monolithic films”, these structures brought about the discussion of the stabilization of electric and elastic domains owing to the presence of very large interfaces in addition to the misfit strain. Roughly the same era also witnessed the rapid advancement in magnetic superlattices that quickly found their way into the modern harddisk drives and became an integral part of the computer revolution. On partial grounds, it appears to be the same motivation to undertake intensive theoretical and experimental studies on ferroelectric multilayer structures as the only difference with respect to the magnetic superlattices was, at first sight, the presence of an electrical ordering rather than spins. However, magnetic superlattices of metallic constituents were mostly studied for their quantum transport properties. Ferroelectrics are considered as insulators and were perceived as candidates for components with capacitive response. Over the course of the years, dramatic differences between the characteristics the ferroelectric superlattices displayed and those of films and bulk were reported. It did not take long to comprehend the complexity of the mechanisms behind the deviation of the phase transition characteristics of ferroelectric superlattices from their monolithic counterparts.

In this talk, I will discuss our work on the phase transitions in ferroelectric-paraelectric superlattices in the light of Landau Theory. It will be shown that the electrostatic and elastic interactions are too strong to ignore compared to intrinsic energy terms and can govern the macroscopic properties. The sensitivity of these structures to electrostatic and elastic boundary conditions will be demonstrated for some limiting and intermediate cases that could in principle allow the “engineering of phase transitions” of these systems towards a desired functionality. With the same token, it will also become apparent why numerous groups report a rich variety of results from these structures that is both the driving force for future work and the apparent confusion in interpreting the results.

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# Measurement protocols for a reliable electrical characterization of perovskite solar cells

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Perovskite solar cells (PSCs) recorded an impressive increase in power conversion efficiencies (PCEs), to date reaching 23.7%. The J-V hysteresis effects, observed since the early investigations of the PSCs, are known to create difficulties for a correct determination of the solar cell PCE. The hysteretic effects depend on several factors, such as PSC poling, scan rate and direction, as well as scan order (reverse-forward vs. forward-reverse scans). Some particular measurement conditions can render an apparent hysteresis-free behavior. In this context, as there are presently more and more reports of hysteresis-free PSCs, it is crucial to determine to what extent the hysteretic effects or their absence are truly related to fabrication methods or are a consequence of the measurement conditions. We discuss here the common pitfalls that may occur in the J-V measurements and propose a set of guidelines for a reliable electrical characterization of the PSCs [1,2]. A large pre-poling voltage can artificially enhance the PCE when a reverse-forward measurement is performed, while a fast scan rate can render the PSC hysteresis-free although the obtained J-V characteristics is far away from the stationary case. Furthermore, independent forward and reverse scans may not always offer a correct assessment of the J-V hysteresis. Furthermore, for a proper characterization of the J-V hysteresis, we define a new hysteresis index, which consistently describes both normal and inverted hysteresis.

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## Very high thermoelectric performances in Sr-doped textured $\text{Ca}_3\text{Co}_4\text{O}_9$ . Costs optimization of unileg thermoelectric generator fabrication.

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In this work, textured Sr-doped  $\text{Ca}_3\text{Co}_4\text{O}_9$  materials, prepared by the classical solid state method and hot-uniaxial pressing, with very high power factor (PF, 1.16 mW/K<sup>2</sup>m @ 800 °C) have been prepared. On the other hand, the Figure-of-Merit, ZT, (0.29 @ 800 °C) is drastically reduced from the expected values due to unusually high thermal conductivity (4.3 W/K m @ room temperature). Even if ZT is lower than 1, this material is still attractive for practical applications. However, the number and duration of processing steps make these materials unaffordable for industrial fabrication. Consequently, it has been necessary to modify the fabrication process to reduce productions costs. In a first attempt, one processing step (24 h @ 900 °C for sintering) has been eliminated, and the effect on thermoelectric performances has been determined. Moreover, the effect of high temperature (800 °C) and time (up to 1532 h) on the thermoelectric and mechanical properties has been studied. After aging evaluation, it has been necessary to reduce, in a larger extent, the processing times using easily scalable processes. With this purpose in mind, a different approach has been used, leading to a reduction of processing times from the original 62 h, to only 2 h. This reduction has led to a decrease in PF values from 1.16 to 0.7 mW/K<sup>2</sup>m. In spite of this PF decrease, the values are still higher than the obtained after the elimination of the sintering step (0.65 mW/K<sup>2</sup>m). These data clearly point out that the decrease in PF values, however, is worth by the drastic reduction of processing time.

Using the materials prepared through the reduced processing process, a new “-type” unileg thermoelectric structure has been designed and tested. This structure, composed with a single thermoelectric material, avoids different thermal expansion coefficients, giving good mechanical strength and increased lifespan during thermal cycling. Moreover, it also avoids the need of soldering at the hot end of the thermoelectric leg.



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## **Power-to-X: the role of catalysis in advancing the electrochemical synthesis of our most coveted chemicals**

**Ifan E.L. Stephens,**

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Our most commonly produced chemicals, such as ammonia, carbon monoxide or hydrogen peroxide are currently produced in large-scale centralised plants. The transport of these reactive chemicals to the point of consumption poses significant safety and logistical challenges. However, with the advent of inexpensive renewable electricity, electrochemical routes of synthesising these chemicals are becoming increasingly attractive.

Low temperature electrochemical devices are particularly amenable towards coupling with renewables. They require little infrastructure; as such, they could allow localised chemical production at the point-of-consumption. Key to controlling the efficiency of these processes is judicious choice of the catalyst at the electrode, i.e. the electrocatalyst.

I will present my research on the electrocatalysis of (i) oxygen evolution (ii) oxygen reduction to hydrogen peroxide and (iii) dinitrogen reduction to ammonia. I will explain the fundamental bottlenecks we face in enabling the large-scale uptake of these technologies, along with a perspective on how we can solve these challenges.

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# Going green with black: On Biomass, Carbon and Clean Energy

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**Keywords:** Hydrothermal Carbonization, Lignin, Biomass Conversion, ORR/OER, Na-ion batteries, supercapacitors

One of the grand challenges facing humanity today is access to sustainable materials and chemicals which are at the heart of sustainable technologies. The production of materials, chemicals and fuels from abundant and renewable resources will eliminate our dependence on petroleum/critical metal-based supplies and will provide access to a new economy based on available reserves.

Carbon is the most versatile element known. It combines with other (carbon) atoms giving rise to new carbon materials with astonishing properties. The versatility and potential of carbon has attracted top recognition in the last decade for the work in fullerenes (1996 Nobel Prize in Chemistry), CNTs (2008 Kavli Prize in Nanoscience) and graphene (2010 Nobel Prize in Physics). However, the mystery and wonder of carbon offers more to discover.

While carbon is widespread on Earth, it has been mainly synthesized from fossil fuel-based precursors with sophisticated and energy consuming methodologies that generate toxic gases and chemicals. The preparation of carbon materials from renewable resources is a key research challenge in terms of sustainability, climate change and economics. Since the beginning Nature created carbon from biomass.

We have demonstrated that it is possible to mimicking the natural process of carbon formation and prepare carbon nanomaterials from biomass using mild hydrothermal processes. Along with amorphous carbon materials (denoted HTC), this procedure also enables biomass transformation into useful chemicals such as 5-hydroxymethylfurfural (5-HMF) or levulinic acid (LA). Recently, we have discovered a third product of Hydrothermal Carbonisation - a crystalline form of carbon - arising at the interface between the amorphous HTC microspheres and the aqueous phase containing the biomass-derived chemicals.

In this talk I will present some of the fundamentals governing the production of carbon nanomaterials and chemicals. We will also discuss the application of HTC materials in electrocatalytic reactions such as Oxygen Reduction Reaction as well as for energy storage in Na-ion batteries and supercapacitors.

Finally, some of the photo-physics governing the optoelectronic properties of the new family of fluorescent hydrothermal carbon nanocrystals will be presented.

**National Institute of Materials Physics**  
**Short presentations**

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# Photoelectron spectromicroscopy: revealing the stability of ferroelectric surfaces with respect to irradiation and contamination

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Ferroelectric surfaces are promising materials for catalysis [1] and photocatalysis [2], mainly due to two reasons: (i) the surface electric field is effective in fixing ambient molecules on its surface [3,4]; (ii) the internal field, manifesting at least near the surfaces of the ferroelectric, enables the driving charge carriers towards the surface, promoting outwards or inwards polarized areas as good candidates for oxidation or reduction reactions, respectively [4,5]. Photoelectron spectroscopy was demonstrated as a principle tool to characterize the surface band bending and to infer in a non-invasive way the polarization of a ferroelectric surface [3].

One step further is to characterize these surfaces by photoelectron spectromicroscopy (microESCA, nanoESCA, PEEM) to infer the polarization landscape of a ferroelectric surface by using the contrast in binding energies of core levels from the material [6,7]. In particular, in some cases areas with uncompensated internal fields are detected, where only progressively charge generation by photoemission builds up the compensating charge sheets [6]. However, in strong radiation fields (vacuum UV or soft X-rays) the ferroelectric surfaces of perovskite type  $\text{ABO}_3$  are degraded with release of neutral A clusters [8]. This degradation is more pronounced on areas with null normal component of the polarization, and a model was proposed involving hot secondary electrons produced by core hole decay in the case of soft X-ray or by direct photoionization in the case of UV absorption. Also, in the presence of polar contaminants, which are known to attach mostly on areas with outwards polarization [4], the surface degradation is much faster; also, in the case of molecular adsorbates (e. g. CO) the strong surface electric field yields a considerable dissociation of them, and subsequent irradiation yields to their partial elimination with uptake of oxygen from the substrate perovskite [3], again, affecting the surface chemical composition.

It is then clear that, for an effective use of ferroelectrics in catalysis, photocatalysis, fuel cells (etc.) all these stability phenomena must be properly taken into account, if possible, by using surface chemical probes such as photoelectron spectroscopy or ESCA with good spatial resolution and with sufficient signal-to-noise ratio to allow the follow-up of these phenomena in real time. This talk will give an account of the actual researches in this field.

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## **Composites based on carbon nanotubes and polydiphenylamine: from the functionalization process to applications in the energy storage field**

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The diphenylamine (DPA) electropolymerization onto the Pt electrode surface covered with a single-walled carbon nanotubes (SWNTs) film in the presence of a semi-aqueous solution of 1M HCl in absence and in the presence of  $\text{H}_3\text{PW}_{12}\text{O}_{40}$  was carried out by cyclic voltammetry. [1,2] The changes reported in the profile of cyclic voltammograms indicate that irreversible processes to take place onto working electrode surface. Using Raman scattering and IR spectroscopy, new arguments concerning the formation SWNTs covalently functionalized with polydiphenylamine (PDPA) doped with  $\text{Cl}^-$  ions and  $\text{H}_3\text{PW}_{12}\text{O}_{40}$  heteropolyanions are shown. [1, 2]

The skinning of the films of SWNTs covalently functionalized with PDPA doped with  $\text{Cl}^-$  ions and  $\text{H}_3\text{PW}_{12}\text{O}_{40}$  heteropolyanions onto the Pt electrodes surface has allowed the prepared of electrodes for the applications in the field of the lithium researchable batteries and symmetrical supercapacitors, respectively. Using as active electrode material in the case of the lithium researchable batteries, a specific discharge capacity of  $\sim 245 \text{ mA h g}^{-1}$  is reported in the case of SWNTs covalently functionalized with PDPA doped with  $\text{Cl}^-$  ions. [1] In the case of SWNTs covalently functionalized with PDPA doped with  $\text{H}_3\text{PW}_{12}\text{O}_{40}$  heteropolyanions, used as active materials in the symmetrical supercapacitors, the discharge capacitance values of  $\sim 157.2 \text{ mF/cm}^2$  were reported. [2]

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## Organometallic compounds for photovoltaic applications

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Organometallic compounds could be an excellent alternative to the organic active layers for solar cells due to several better properties like thermal and chemical stability. These organometallic compounds are electron donor materials which are easily used in donor-acceptor heterojunctions in these solar cells.

One of the main problems for the active media in the solar cells is connected with the exciton diffusion length which limits the thickness of the donor layer in these donor-acceptor heterojunctions. A way to improve the exciton diffusion length is a better charge transfer between the donor and acceptor facilitating the exciton diffusion towards the electrodes of the solar cells. The adding of electronegative ions or chemical groups could also influence the band alignment between the donor and acceptor smoothing the charge transport across the solar cells.

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# Nanotechnology of Pinning Centres in Superconducting Films for Clean Energy-saving Power Applications

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Energy resources are now a major issue in the global economy, while climate changes due to increasing CO<sub>2</sub> emissions are now obvious. In these circumstances, a large number of devices and equipment with increased energy efficiency and more environmentally-friendly, based on advanced superconducting materials, will start, gradually, to replace the existing "classical" devices and equipment. Even now, a large number of magneto-superconducting equipment cooled below liquid nitrogen temperature proved to be highly energy efficient (50% less consumption) and environmentally-friendly and with a longer lifetime compared with their copper-based counterparts: magnetic billet heaters for non-ferrous metallurgy, superconducting-magnetic energy storage, fault current limiters, superconducting electric engines for ship propulsion and wind turbines, transformers, superconducting cables for large currents, etc..

From economics point of view, larger market penetration of cryo-electro-magnetic devices fabricated from superconducting bulk/wires/tapes) depends on the cost, expressed in Euro/kA·m, hence, the price reduction can be achieved by increasing the critical current  $I_c$  (maximum current that can be transported without losses).

High magnetic fields strongly reduce critical current density due to the dissipation caused by the movement of flux lines (Lorentz force, thermally-activated flux creep). The above-mentioned dissipation can be minimized by artificial defects (nanostructuring) that could fix (pin) the magnetic flux lines due to the decrease in the free energy if the flux line "sit" on the defect. In the case of YBa<sub>2</sub>Cu<sub>3</sub>O<sub>x</sub> high-temperature superconducting films, nanotechnology of pinning centres involves several approaches: substrate decoration, quasi-multilayers and multilayers, targets with secondary phase nanoinclusions, and combinations of the above mentioned [1-4], involving various architectures and nanoinclusions. We will present results from DC magnetization loops, magnetic relaxation, AC susceptibility and TEM images and discuss the improvements in critical current for various nano-architecture. The difference between correlated and synergetic pinning centres are also very important and will be pointed out.

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## Cost efficient oxygen generation through alkaline water electrolysis using Ni on SnO<sub>2</sub> mesoporous support-based electrocatalysts

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Developing highly efficient and cost effective electrocatalysts for water oxidation is a tremendous challenge of these days, due to increasing worldwide energetic demands in the last decades. In this study, we report a general deposition-precipitation methodology for the synthesis of a well-dispersed Ni-based electrocatalyst on bimodal mesoporous SnO<sub>2</sub> support material. These composites can catalyse the oxygen evolution reaction under alkaline conditions without any other modification of the compositional phases or doping with noble metals. The powders have been characterized by adsorption-desorption isotherms, TG-DTA, XRD, SEM, TEM, Raman, TPR-H<sub>2</sub>, and XPS.

The best NiSn composite can generate, at extremely low quantities (approx. 3.78 ng) of Ni species, more than 3.6 mA cm<sup>-2</sup> at an overpotential value of approx. +0.33 V vs. RHE. Under these experimental conditions, a turnover frequency value higher than 1.14 s<sup>-1</sup> and a mass activity higher than 370 A g<sup>-1</sup> has been obtained, which is a remarkable result considering the low amount of electrocatalyst used in the preparation of the composites. We demonstrate, by the means of different techniques, the importance of the synergy created between SnO<sub>2</sub> and Ni species. In the light of these findings, NiSn composites can be seen as potential candidates for practical applications.



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## "Development of thermal barriers materials with application in energy"

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Metal-ceramic composites have been developed by a powder metallurgy route to control the heat flow through components exposed to high temperatures. Depending on the materials used such components can operate at temperatures over 1000° C and act as thermal barriers creating temperature gradients of several hundreds of K over distances less than a millimetre. Due to the large compositional range possible (up to 90% ceramic content volume) the thermophysical properties (like thermal conductivity, specific heat, thermal expansion coefficient) can be easily tuned to designed values and due to the metal presence in the composite, the resulting thermal barriers can also be joined or embedded in components. The materials retain a metallic electrical conductivity while having thermal conductivities even below 1 W/m/K, lower than usual ceramic materials.

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## Improved performance of a Si-solar cell by up-conversion in Yb/Er doped CeO<sub>2</sub> thin films

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At the end of 2016, about 315 GW of power was generated by PV technology, and according to market forecasts, it could double by 2019. Worldwide solar PV power is expected to exceed 400 GW in 2017, thus being capable to produce 2 % of electricity demand. In EU, the share amount is about a quarter of the world-wide installed capacity, providing about 4 % of electricity demand [1]. The Si-wafer-based PV technology accounted for up to 94% of total production in 2016 [2].

Thin films of Yb/Er - doped CeO<sub>2</sub> were grown on a p+-n-n+ single crystal silicon diode. The bulk target composition was Ce<sub>0.95</sub>Yb<sub>0.04</sub>Er<sub>0.01</sub>O<sub>2</sub>. Thin films were deposited by pulsed laser deposition (PLD) with a fluence ranging between 1.7 J/cm<sup>2</sup> and 3.7 J/cm<sup>2</sup>. The optimum growth condition was found for a laser fluence of 2.3 J/cm<sup>2</sup>. This film shows the best target-film composition transfer, a granular morphology and the lowest roughness. Under 1 and 2.1 sun illumination, the as fabricated device shows an increase in relative power conversion efficiency of 12.1 % and 38.9 %. Under 980 nm light, the increase of relative external quantum efficiency was 8.2 %. The mechanism responsible for improvement is based on efficient energy transfer between spatially separated Yb<sup>3+</sup> and Er<sup>3+</sup> ions.

\*Authors acknowledge the financial support from MCI-UEFISCDI, Core Program 2017/2018. ME and PB also acknowledge POC 37\_697 no. 28/01.09.2016.

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## Reticulated mesoporous TiO<sub>2</sub> scaffold for hybrid perovskite solar cells

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Perovskite solar cells (PSC) shows the fastest advance in solar technology to date. This happens due to the hybrid perovskite material's properties that translate directly in devices with very high power conversion efficiency (PCE). Additionally, because they are processable from solutions, present significant possibilities for low-cost, industry-scalable technology. Although most of the perovskite solar cells components are already optimized, there is room for improvement, especially when scaling to large area is foreseen. And although there are claims of fully printable PSCs, the mesoporous TiO<sub>2</sub> scaffold was severely overlooked, being still fabricated by conventional small area methods [1], [2] even for devices with larger active areas.

We report the successful fabrication of large area mesoporous TiO<sub>2</sub> scaffold by a spray coating technique. Our mesoporous presents a specific reticulated structure with well-delimited, irregular shape cavities of diameters in the range of 3 to 7 µm, ~ 350 nm height and increased roughness of ~150 nm that proved to be beneficial for PSCs. We study the effects of integrating such structure in PSCs and compare the results with devices where the mesoporous TiO<sub>2</sub> was fabricated by conventional spin coating. We show that this specific reticulated structure improves the efficiency and the reproducibility of PSCs.

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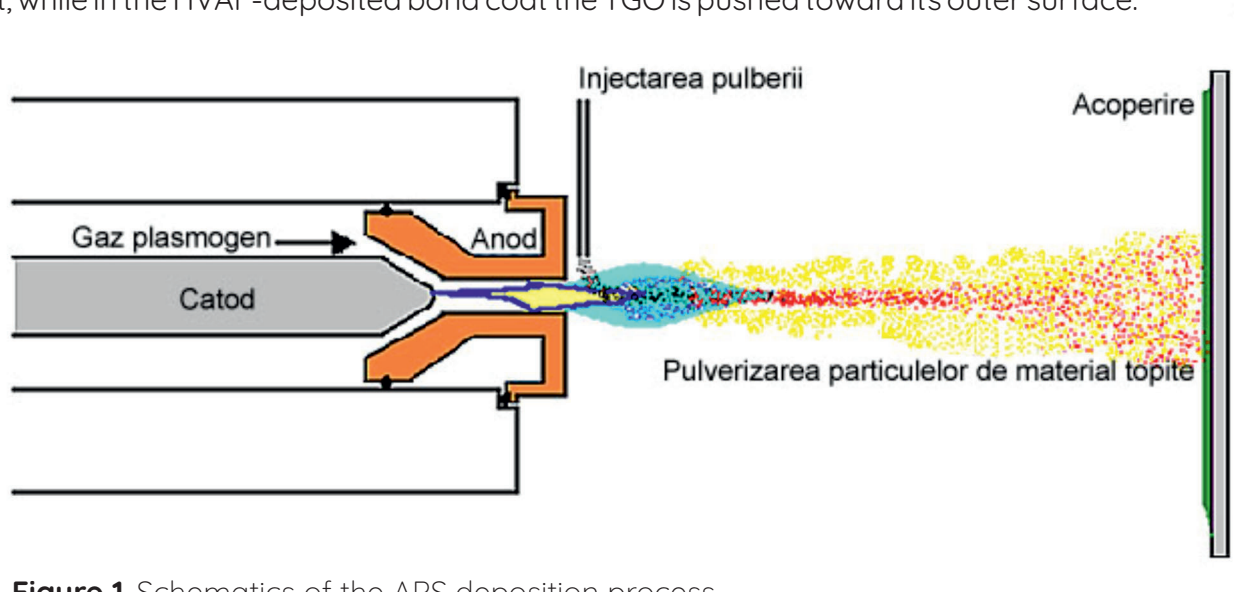
# On the adherence of ceramic layers for thermal barriers coatings

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Thermal barrier coatings (TBC) represent the most effective system to protect structural components from damage caused by high temperature and corrosive/erosive environments. Yttria-stabilized zirconia (YSZ) is among the most studied ceramics for such applications. The adherence of the ceramic layer to the metallic object needing thermal protection is one of the critical issues in real operation conditions at high temperature or under thermal shocks. A bond coat is necessary to ensure the adherence of the YSZ top coat to the substrate. In our work, Y, Ta doped NiCrAl compounds bond coat obtained by air plasma spray (APS – Fig. 1) and high velocity air fuel (HVOF) have been subjected to increasing temperature thermal treatments (700 – 1300 °C/5 h). The system behavior under thermal stress has been investigated by microstructural methods including XRD, SEM and TEM. The TEM/STEM results (Fig. 2) show the oxidation resistance of the HVOF vs APS deposited bond coats. Spurious Y-Ta-O structures have been evidenced which otherwise failed to be observed by conventional XRD/SEM-EDS (Fig. 3).

The identified microphases which appear at the high temperature represent the nucleation point for the layer of thermally grown oxide (TGO) with a decisive role in the delaminating process at high temperature. We show that in the APS-deposited bond coat the TGO was distributed in the whole mass of the bond coat, while in the HVOF-deposited bond coat the TGO is pushed toward its outer surface.



**Figure 1.** Schematics of the APS deposition process.

## Conclusions:

- Formation of TGO is initiated both at the ceramic-bond layer interface and into the pores existing inside the bond layer.
- The size and morphology of the pores inside the deposited layers depend on the deposition method (ex: APS or HVOF).
- Fracture occurs at the YSZ/TGO interface.
- Below fracture, the TGO to bond coat transition is abrupt (~ 5 – 10 μm).

- Diffuse  $\text{Al}_2\text{O}_3$  can be observed in TGO/BC region (2), which segregates at the BC/substrate interface (3); TGO does not built in a compact oxidation barrier layer.
- Ta, Y, Ti segregations form into the top coat, bond coat and substrate.

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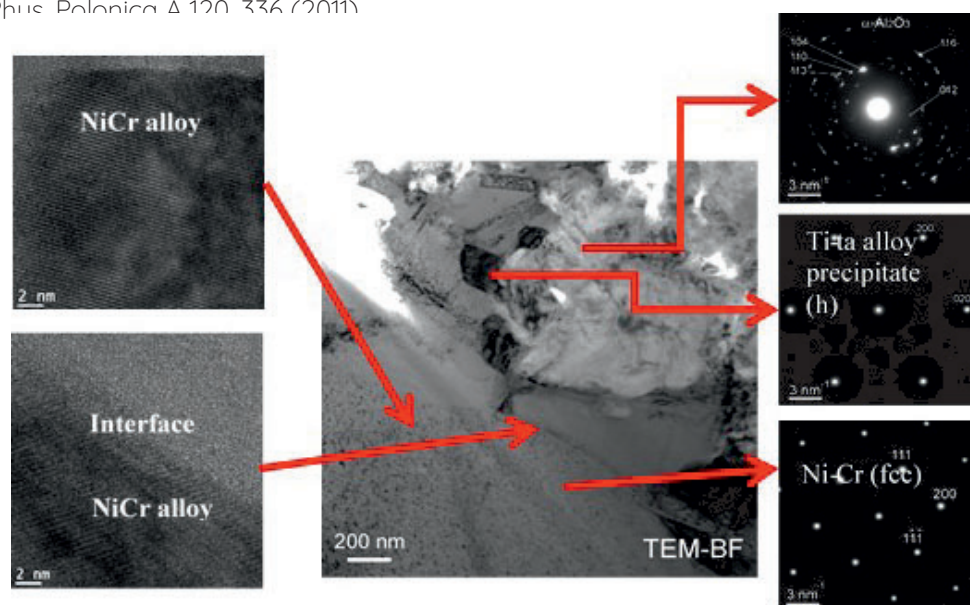
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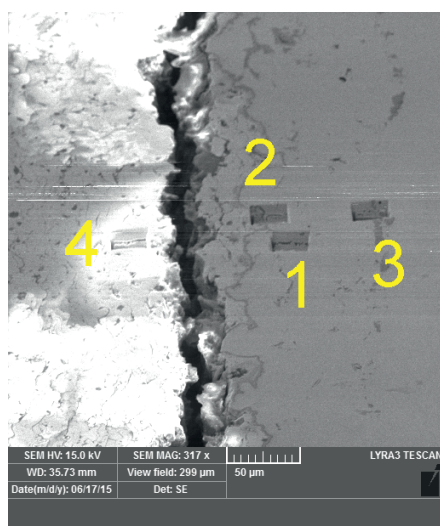
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**Figure 2.** TEM, HRTEM and SAED identification of the TGO phase.



**Figure 3.** Cross-section SEM image indicating the spots from where thin lamellas have been extracted around the TBC-substrate interface for TEM investigations: 1- bond coat (BC); 2 - TGO/BC; 3 – substrate; 4 - top coat.

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## The use of three-component composites in the photocatalytic water splitting reaction

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In the framework of semiconductor photocatalysis, water splitting is among the most studied reaction, with TiO<sub>2</sub> Evonik P25 standing as reference material for such application. Starting from the first glorious moment of electrochemical photolysis of water at a semiconductor electrode done by Fujishima and Honda in the year 1972, a new worldwide research era begins. Basically, this study was considered the cornerstone of photocatalysis and from this moment enormous effort has been done and thousands of studies performed. However, the preparation of efficient materials able to produce molecular fuels at a competitive scale and cost, remains a significant challenge for all the scientists working in fields ranging from materials science to physical and inorganic chemistry and particularly photocatalysis.

Starting from the moment when Bard introduced the concept of pairing semiconductors for water splitting much effort has been made to develop active photocatalysts. A p-n junction is an interface between two different types of semiconductors. In the interface, the energy bands are bent and the Fermi levels are adjusted to reach a new balance between diffusion and migration, which results in the formation of a space-charge region. Built-in potential in this region enables the effective separation of the mobile carriers. Although most of the studies imply the pairing of two semiconductors, the preparation and optimization of three-component structures should create great opportunities for further improvements.

Starting from this premise, this study provides a significant advance on the synthesis, characterization and the photocatalytic performance of a new highly efficient Ni-Zn/TiO<sub>2</sub> ternary composite system. The use of ternary composites is an original aspect of this work, since is scarcely reported in the literature. The advantages of this study are the following:

- i) These composites can be prepared through a simple and reproducible low-cost synthetic technique such as the deposition-precipitation of the Ni and Zn nanoparticles onto the surface of TiO<sub>2</sub> Evonik P25;
- ii) From the XPS analysis and theoretical aspects about the band alignment for ZnO/TiO<sub>2</sub>/Ni heterointerfaces we can conclude that the TiO<sub>2</sub> becomes degenerated semiconductor, accumulates electrons and under UV irradiation tunnels these electrons to the Ni nanoparticles, while the holes are directed to the ZnO;
- iii) The samples present very good photoactivity under UV light irradiation condition. For instance, the most active synthesized composite exhibits H<sub>2</sub> generation rate above 17000 μmols g<sup>-1</sup> h<sup>-1</sup>, which is nearly one thousand times higher than that obtained with TiO<sub>2</sub> Evonik P25. The remarkable photocatalytic properties of composites associating TiO<sub>2</sub> with both Ni (oxidized) and ZnO points on effective electron-hole separation, which may be achieved by using local heterostructures.

Nevertheless, this work demonstrates not only the capability of these ternary composites to efficiently split the water photocatalytically, but provides insights in surface science, demonstrating the band alignment for ZnO/TiO<sub>2</sub>/Ni at local heterointerfaces and the formation of degenerated TiO<sub>2</sub> type semiconductor in this case.



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# Carbon monoxide adsorption, dissociation and oxidation on ferroelectric surfaces decorated with nanoparticles of noble metals

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Surface reactions involving carbon monoxide are of actual interest since almost a century, owing to the harmfulness of this molecule, the necessity to remove it from the exhaust gases, or to convert it into fuels via Fischer – Tropsch synthesis or methanation [1]. An important point regards the fixation of this molecule on the surface of a catalyst, together with the ability to dissociate it and to ensure a sufficient surface mobility of the resulting fragments [2]. Chemical and catalytic activity of ferroelectric surfaces is an actual area since more than one decade [3]; however, concerning carbon monoxide, only recently experiments have been performed in ultraclean conditions on well-defined surfaces from both stoichiometric and structural points of view, with well characterized polarization orientation and follow-up in real time of adsorption/desorption processes [4]. The main results of this study were (i) a straightforward correlation between the amount of carbon monoxide adsorbed and the polarization state of the substrate, (ii) evidence for considerable dissociation of the molecule upon its fixation on the ferroelectric surface; (iii) the carbon release in the form of CO<sub>2</sub> with temperature increase up to the loss of the surface ferroelectric polarization.

Actual catalysts for CO-related reactions are noble metals (Pd, Pt), owing, amongst others, to the complex charge transfer (donation from □ electrons to the metal, back-donation of d electrons from the metal into antibonding □\* orbitals) occurring when CO is adsorbed on these metals [1]. A natural choice is to combine noble metals with ferroelectric surfaces and, indeed, the first results were quite promising, e. g. in achieving a rate of almost 100 % CO oxidation at temperatures as low as 350 K [5]. Also, noble metal (Au) nanoparticles were detected in negatively charged states upon their deposition on ferroelectric surfaces [6] and one expects that these charge states will drastically influence the back-donation and hence the dissociation pathways of adsorbed molecules. These results and expectations encouraged us to reproduce the results from Ref. [4] by using ferroelectric surfaces pre-decorated with Au or Ag nanoparticles. An enhanced amount of CO adsorption, an improvement of relative amount of dissociated carbon together with a clear evidence for desorption in form of carbon dioxide were detected. Time-resolved photoelectron spectroscopy (TR-XPS) was the principle tool to investigate these phenomena, but the surfaces were characterized also by scanning tunneling microscopy (STM) and by atomic and piezoresponse force microscopy (AFM, PFM).

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## “Thermoelectric nano-composite from double filled skutterudite and carbides”

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Double filled  $\text{In}_{0.2}\text{Yb}_{0.2}\text{Co}_4\text{Sb}_{12}$  skutterudite based composites with various volume percentages of  $\beta$ -SiC or WC nanoparticles dispersions have been processed using a melting – annealing - ball milling - spark plasma sintering route. XRD/EDX and SEM investigation are used to determine the structural and morphological properties of the specimens. Samples with suited geometry have been investigated to characterize the transport properties at temperatures up to 600 °C. Low content of  $\beta$ -SiC leads to increased electric conductivity, Seebeck coefficient and thermal conductivity and to an approximately 10% increase of the figure of merit at about 450 °C, as compared to the bare skutterudite material.

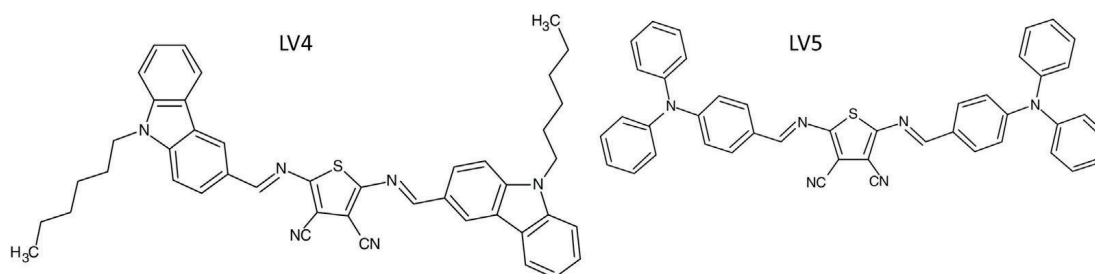


# Tryphenylamine and carbazol oligomers for photovoltaic applications

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Nowadays, there is an increase interest in the conductive organic materials for photovoltaic applications due to their manufacturing process malleability. An important step is the synthesis of new donor/acceptor materials which can enhance the performances of the organic solar cells. In this context, we present studies regarding the properties of mixed layers containing tryphenylamine (LV4) and carbazol (LV5) oligomers as donors and a fullerene derivative (PCB-C4) as acceptor prepared by Matrix Assisted Pulsed Laser Evaporation (MAPLE) on ITO or silicon substrates. The effect of the weight ratio between the donor and acceptor (1:1; 1:2) and the solvent type (chloroform(Ch) or dimetylsulphoxide (DMSO)) on the optical, morphological and electrical properties have been investigated.



Chemical structure of utilized compounds

The results have highlighted that chloroform is more adequate to use in the MAPLE process for film deposition. The mixed layers show a good transparency over 600 nm, and a strong quenching of the emission at UV-vis excitation.

The I-V characteristics pointed out that the structure ITO/LV5:( PCB-C4) (1:1) prepared using chloroform as solvent have the higher dark current, short circuit current and fill factor from all the realized heterostructures.

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