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Welcome to the Thinface Newsletter 3

Many of you will look forward to the upcoming Summer School at Como in Italy in September.

More than 120 participants have demonstrated their interest in the topics on Organic Electronics and also in the wonderful place. It will be the 7th School organized by PCAM and this time together with Thinface. Check out the program .

Another highlight will be the the conference on 'Smart Materials and Structures' in Marrakech, offering a Thinface workshop which deadline for submissions is July 5. The conference is in September. Visit the homepage here.

And yet one more important date for the Thinface Network will be the Mid Term Review on August 20, 2015 in Brussels.

Apart from this short Outlook the Newsletter offers some more interesting articles:

PCAM* certificate for European doctorate in Materials Sciences

Dear ESR students, this is a chance to obtain an extra certificate on your PhD.

The main purpose of this project is to offer scientific, competitive education and research training at the doctorate level in a European context. All 15 member universities** agree to provide, when possible, an additional certificate stating the European value of their doctorate. The following rules apply:

- Fulfill the requirements of your home institution
- Join any of the doctorate programmes of PCAM members **
- Spend a minimum of six months with at least one of the PCAM universities.
- Supervision should be organized of senior academic staff from the involved universities
- Present thesis in English
- A member of a PCAM university, will be appointed to be a member of the jury.
- The student has to attend at least one PCAM summer school and pass (with grades) one exam with at least one examiner from the universities signing the present Partnership Agreement (listet in **), but not belonging to the home university, on a topic of the summer schools or any course or seminar attended in the guest universities. Exams may be taken by email.
- Before the final oral exam, the doctorate thesis will be evaluated by two foreign scientists not belonging to the home university.

In case you are interested and would like some more details, please contact Katharina Rubahn (kru@tek.sdu.dk)

*Physics and Chemistry of Advanced Materials, http://www.pcam-doctorate.eu/
** Universita` Degli Studi di Milano-Bicocca, Universidad Autónoma de Madrid, University of the Basque Country, Universita`Degli Studi di Milano, University of Southern Denmark, Jagiellonian University, Kaunas University of Technology, Université Pierre et Marie Curie, Carl v. Ossietzky University, M.V. Lomonosov Moscow State University, Technical University of Cluj-Napoca, Graz University of Technology, University of Liverpool, University of Luxembourg, Technische

Laura Calio introduces herself and her work on Perovskite Solar Cells

Laura Calió, originally from Italy but currently working at Abengoa Research, Spain, thanks to the European Union Marie Curie program, which allows young researcher like me to not only learn new things but also to adapt new culture. Abengoa is a world leader in solar thermal technology and second in biofuel generation, a company fully dedicated towards energy and environment. One of the main projects in Abengoa Research is perovskite solar cells. Abengoa Research and the team of Shahzada Ahmad are working in this direction since its

genesis in 2012.

My research interest in this project in the framework of "Thinface" is in depth study on the structure and the peculiarity of hybrid solar cells with new materials. I work in the area of nano-structured solar cells in general and perovskite solar cells in particularly.

Organometal halides $CH_3NH_3MX_3$ (M=Pb, Sn; X = Cl, Br, I), are receiving great attention due to the panchromatic light absorption and ambipolar behavior. Perovskites act as a pigment as well as they create electron and hole pairs. In less than three years the light to electricity conversion efficiencies have reached over >20% in solid-state hybrid solar cells. The record certified efficiency is 20.1%, which is very close to the mature thin film based photo voltage technology. Now that the efficiency of the devices reached such a good level, the interest turned toward improving the stability of the devices and lowering their cost, in order to make them feasible for commercialization.
So my work in the first 6 months was focused on the fabrication of full devices, from the synthesis of the organic salts forming the perovskites to the preparation of each of the thin films forming the devices. Every layer is very important for the efficiency of the full device, so I'm trying to change and improve every single layer to find the best configuration possible. I'm now focusing on the two step process of the perovskite formation, and in particular in changing the ratio of the organic salts (methylamonium and formamidinium iodide) that form the perovskite, i.e. the absorber in the solar devices. The deposition of the perovskite is quite water sensitive, so this process has to be done in a glove box or dry box which has controlled atmosphere. In the picture you can see me working in the glove box during the fabrication of a new batch of Solar Cells.
Furthermore I'm focusing on the exploration of new dopant for the Hole Transporting Material, i.e. Spiro-OMeTAD in order to improve the stability of the Solar cells. Currently lithium salts are used for doping Spiro-OMeTAD to increase their charge carriers and make them suitable for device fabrication; however lithium salts are very hygroscopic and thus induce instability in devices. My task is

to fabricate stable devices without compromising the efficiency of the devices. Beside this I'm also developing new small organic molecules which are cost effective for the possible replacement of expensive Spiro. So I'm also focusing on the organic synthesis and the characterization of brand new organic molecules that could be feasible as cheaper and hopefully better Hole Transporting material for the perovskite solar cells.

Meet Weike Wang

Hi, my name is Weike Wang, from Shanxi province, China. I studied at Taiyuan University of Technology during my master period, focusing on the gas chemisorption of Metal organic framework materials (MOFs). My research interests involve synthesizing MOFs and using various ways to modify these materials so that new interesting properties arise. Since July 1st, 2014, I have started my Ph.D project at CIC nanoGUNE, Donostia-San Sebastian, Spain, as a member of Dr. Mato Knez group. I am investigating a vacuum based process (atomic layer deposition-ALD) for the top-down synthesis of conducting polymer-inorganic hybrids.

On February 26,2015, I went to the Institute of Coal chemistry, Chinese Academy of Sciences in Taiyuan, China, and visited the ALD lab of prof. Yong Qins group. Yong and I talked about my project and the collaboration possibilities using ALD and MLD (molecular layer deposition) to modify the nanoparticles and polymers.

Besides the science I love playing pingpang, hiking, reading chinese classical novels, and enjoy very much traveling. If you have an interest in my project, please contact me, never hesitate.

Vapor phase doping and infiltration of conducting polymers introduced by Weike Wang

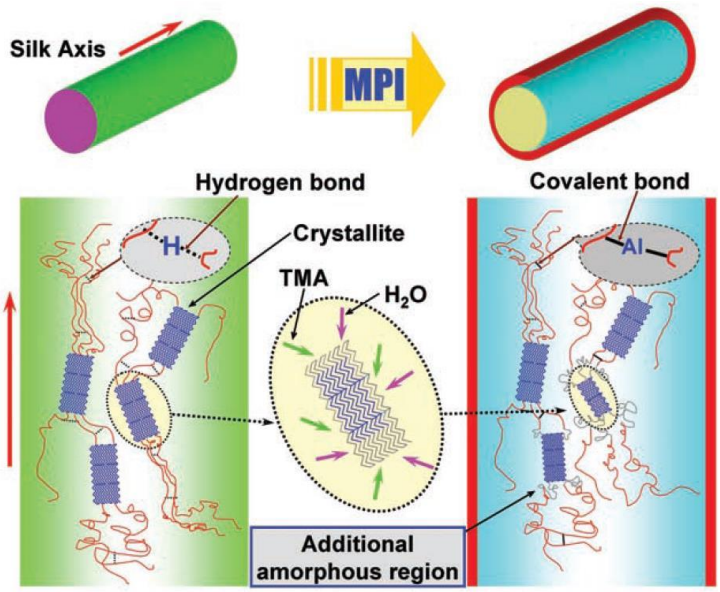

Fig.1 *Schematic description of proposed molecular changes in the silk produced by* MPI *(thin film deposition plus chemical modification by metal infiltration).* [1]

The aim of this project is to exploit a vacuum based process (atomic layer deposition – ALD) for the top-down synthesis of conducting polymer-inorganic hybrids. Although ALD is commonly seen a thin film deposition method that results in coatings of substrates with nanoscale films, a modified procedure of the deposition process applied to soft matter results in diffusion of the metal containing precursors into the bulk of the soft substrate[1-3](Fig.1). Such homogeneous incorporation of metals into polymers without undesired side effects induced by the solvents will enable to alter the physical properties of the hybrid in a way complementary to the common routes such as, composite formation through blending of the polymer with inorganic nanoparticles, etc.

The modified ALD process will, dependent on the chemical nature of the metal source (organometallic, metal-organic or halide), allow incorporation of the metal into the polymer and chemical interaction with the backbone and thus an alteration of physical properties. The resulting materials will strongly differ to the commonly synthesized materials as the applied procedure gives access to an entirely new class of hybrid materials, which will be of great impact for emerging applications.

This project is initially focusing on the fundamental understanding of the interactions of the metal-organic precursors with the functional sites of polyaniline (PANI), the impact the interactions have on the conductivity of the material, and finally the possibility to tune the resulting properties by adjusting the parameters for the metal infiltration.

PANI is an organic semiconductor by virtue of its highly conjugated π-delocalized molecular backbone. The application range is very wide and includes electrochromic devices, drug delivery, sensor applications, and rechargeable

batteries[4-6]. These applications generally depend upon the switching between the different states of the polymer, namely, leucoemeraldine, emeraldine, and pernigraniline states[5,6], as a response to chemical or electrical trigger. The present work mainly attempts to achieve enhanced doping of PANI (emeraldine) using the aforementioned infiltration method, in order to achieve higher electrical conductivities than with traditional routes. Several metals such as, Titanium or Tin, have been infiltrated into PANI, resulting in good conductivity of the resulting organic-inorganic hybrid polymer.

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[2] S. M. Lee, V. Ischenko, E. Pippel, A. Masic, O. Moutanabbir, P. Fratzl, M. Knez, Adv. Funct. Mater. 21, 3047 (2011).
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You know our ESR representative Shashank Harivyasi?

Hi, I am Shashank Harivyasi from Dehradun, India. I studied Nanotechnology for my Master's at Amity University in India. My current interest lies in applying quantum mechanical simulations to find materials and device architectures that address real world challenges. What drives me on a daily basis is ability of these simulations to quantify and dissect often complex phenomena allowing for great insight and to answer the question: what's really going on? In the THINFACE project, I am working at the Graz University of Technology under the guidance of Prof. Egbert Zojer. Here, cuddled by the beautiful Alps, we are exploring new interfaces between organic molecules and inorganic substrates since such interfaces form an indispensable part of any organic electronic device.

Beyond science, my interests include history, sociology and philosophy. I also like reading, writing and visiting places. Get in touch if you are interested in my

project, share my interests, have any queries/ideas or if you are visiting Graz and want some company for coffee.

Self-assembled organic structures on metal-oxide layers for organic photovoltaics, Shashank Harivyasi

Exploiting the foundations of traditional electronics, organic electronics has moved quickly from being built at small scale in the laboratory environment to being fabricated in bulk at industrial scale, that is, it has quickly made the 'lab-to-fab' transition. The demand for consumer electronics, such as handheld devices and large flat display panels, has greatly fueled the research of light-emitting technologies. On the other hand, research in the field of light-harvesting technologies such as photovoltaic cells has been slower. However, development of cheap and efficient photovoltaic devices is necessary for a post-fossil-fuel world. [1] Moreover, a fundamental level understanding of organic devices refined particularly to exploit the exclusive advantages of organic devices is still lacking.

Two-dimensional materials, most famously graphene, have shown a number of promising phenomena that can improve/complement current technologies. Building on this promise, a number of layered metal oxides that have been known for decade are being now explored in detail. [2]

In this project, we at the Graz University of Technology explore the interactions that take place at the interface between layered metal-oxides and organic molecules using density functional theory. The first goal of the project is to overcome the challenges related to simulating layered semiconductors some of which are intrinsically doped (as a result of vacancy defects) in their natural state giving rise to altered properties [3]. Following this, the second goal is to understand the interaction between the surfaces of these semiconductors and specially designed molecules that complement these surfaces. The third objective of the project is to specifically target applications in photovoltaics. The project includes two secondments: one at University of Southern Denmark (SDU) under Prof. Jakob Kjelstrup-Hansen and Prof. Morten Madsen where we would try to fabricate solar cells based on the insight gained from our simulations; another at University of Milano-Bicocca under Prof. Gian Paolo Brivio where we will use complementary quantum-mechanical modelling techniques to specifically treat disordered systems.

Figure 1. The layered semiconductors of our interest: MoS_2 (left) and MoO_3 (right). In both cases, molybdenum is red and the chalcogenide is blue.

1. There are several reviews on the current state and role of Organic electronics. For example see: Forrest S. R., *Nature* **428**, 911-918 (2004) | doi:10.1038/nature02498
2. Butler S. Z. *et al*, *ACS Nano* **7**(4), 2898-2926 (2013) | doi:10.1021/nn400280c
3. Balendhran S. *et al*, *Adv. Funct. Mater.*

Instrumentation: Vienna Scientific Cluster 3

Vienna Scientific Cluster 3 (VSC3) is a high performance computing (HPC) system jointly owned by TU Graz and four other Austrian universities. It is a modern parallel computing system with 2020 nodes, each equipped with 2 processors (Intel Xeon E5-2650v2, 2.6 GHz, 8 cores) of the Intel Ivy Bridge family and inter-connected with an InfiBand fabric. VSC3 is one of the 100 fastest computing facilities as well as one of the greenest on the planet. After a phase of extensive testing, it was opened for scientific projects at the beginning of January 2015. More information can be found at http://vsc.ac.at/systems/vsc-3/. One of the projects approved at the VSC3 was exclusively for the needs of THINFACE researchers of TU Graz. The availability of such a high performance system has greatly boosted the pace of research because it has allowed simulation of modelled systems that were previously too big for the TU Graz resources and is, as per internal problem-specific testing, around twice as fast as the previously used resources. Image © VSC / Claudia Blaas-Schenner

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New Publication:
Tuning the optoelectronic properties of amorphous MoOx films by reactive sputtering (1)

The underlying question to our publication is to see whether it is possible to modify the optical and electrical properties of Molybdenum oxide thin films by changing the concentration of oxygen in the film. We used DC sputtering for the deposition of Molybdenum oxide layers. By changing the oxygen partial pressure from

$1.00x10^{-3}$ mbar to $1.37x10^{-3}$ mbar we observe that not only the conductivity varied from 1.6x10-5 S/cm to 3.22 S/cm but also by looking at the transmission and absorption spectrum, the film showed drastic changes. The transparity varied from nearly 50 % to quasi-opaque in the range of 2.00 - 3.5 eV.
To detect the concentration of oxygen in the film, TEM method was performed at Universidade Federal do Rio Grande do Sul and it confirms that we varied the oxygen ratio Table I.

		[O]/[Mo] ratio			
Power (W)	**$1.00x10^{-3}$ mbar pO_2**	**$1.98x10^{-3}$ mbar pO_2**	**$2.7x10^{-3}$ mbar pO_2**
100	3.16	3.16	3.16
150	3.16	3.16	3.16
200	3.00	3.16	3.16
250	2.57	3.16	3.16

Table I- Summary of the [O]/[Mo] ratio measured by Rutherford Backscattering Spectroscopy (RBS) of the MoOx films formed at different oxygen partial pressures and at different sputtering powers.
Contact: Mehrad Ahmadpour

Bibliography: A.L. Fernandes Cauduro, Z.E. Fabrim, M. Ahmadpour, P.F.P. Fichtner, S. Hassing, H.-G. Rubahn, and M. Madsen, Appl. Phys. Lett. **106**, 202101 (2015).

On April 09, 2015, Graz University of Technology organized “Tag der offenen Tür” – an open day for high school students to provide them with an insight of the higher education system and the vast possibilities that await them once they receive technical education. The event had a high footfall and the Inffeldgasse campus of the TU was crowded with students from across Austria since TU Graz is one of the largest technical education institutes in the country. Depending on their interests, students chose freely from numerous sessions held by different departments of the TU.

We were part of a team that was in charge of dispensing information about technical physics and possible areas of physics that one might opt. The session began with a talk by Prof. Roland Würschum, the Dean of Studies for Technical Physics. He motivated the students by talking about the role of physics and physicists in the society, state of modern research and how research in physics leads the current technological revolution. He highlighted how TU Graz is closely linked with a number of industries – especially the automobile, paper and hydropower industries in Europe – making the graduates of the university highly employable. He also talked about non-conventional careers available for holders of a physics degree such as finance, administration and management, areas where the skills of analytical thinking are much valued.

Following this was a talk by Shashank Harivyasi, a THINFACE doctoral student at the TU Graz. He talked about the internationalization of science, and of physics in particular. He stressed the vast number of opportunities that are available to the students in Europe in form of the Erasmus exchange program, Marie Curie research grants, the freedom of movement – both academic and geographic (in light of ECTS system) – and a world-class infrastructure for conducting research. He discussed the differences he felt between the European and Indian technical education system and shared his personal experience of moving to a foreign land, exploring a new culture and learning a new language.

The session was then concluded with an interactive session hosted by Iris Hehn, also a doctoral student at the TU Graz. She focused on a student’s perspective of studying technical physics, discussing the small but important details of day to day activities such as lectures, curriculum, work load, student assistance services and social aspects of a student’s life. She emphasized on the “Frauen in die Technik” policy of the university which encourages active participation of women in sciences and highlighted the number of scholarships and positions that benefit women students and faculty of the university. She also discussed the advantages of undertaking an Erasmus exchange semester and how it works seamlessly with the TU system. With her cheerfulness, she successfully motivated students to openly discuss their doubts and reservations, answering individual questions till the closing of the session.

Shashank Harivyasi

Image © Sporer / TU Graz

Lab Tour at TU Dresden

On May 26th 2015, Bachelor Students from TU Braunschweig were visiting the Institute of Applied Photophysics (IAPP) of TU Dresden for an information event on the possible master's programmes and researching possibilities offered at the IAPP. After an introduction of the institute and its fields of research by the head of the Institute Professor Karl Leo, covering the basic principles of OLEDs, OTFTs and Organic Solar Cells, the students had the possibility to explore the IAPP during a guided lab tour, where they were able to have a look at the different experimental facilities to produce and characterize organic opto-electronic devices. While the evaporation systems for fabricating organic thin films caught most of the attention of the students, some were also interested in hearing the story on how an Austrian came, thanks to the Thinface Project, to Dresden for doing his PhD.

Bernhard Nell

Activities for the THINFACE Science day at Campus Tønder and SDU, Sønderborg, April 2015

Presenters:
Golnaz Sherafatipour, Mina Mirsafaei, Mehrad Ahmadpour
THINFACE fellows at Mads Clausen Institute, SDU, Sønderborg

Thursday and Friday 23rd and 24th of April 2015 were two days in the science week in Denmark, which were dedicated to the topic of light and introducing the green energy sources. On these days, school pupils attended in different programs in this matter at Campus Tønder in Tønder and Alsion, SDU in Sønderborg, Denmark. On 24th afternoon, a light and laser show program was performed by the optic group from Mads Clausen institute, and afterwards we, as Marie Curie ambassadors, ran a booth about solar cells, in which we presented different types of solar cells (e.g. Si, thin film and organic solar cells), and their applications. Moreover, there were solar cell models, devices and short movies to make the learning process more tangible. Among other interesting ingredients, we presented two posters; one describing the fundamental of solar cell and their application, “Collect your energy everywhere, organic solar cells anywhere”, and the other depicting the mission of THINFACE, introducing our site in SDU in Sønderborg and a short description of our projects”Thin film hybrid interfaces, A training initiative for the design of next generation energy devices”. In total, we shared the sprit of science with visitors including some professors from different divisions and more interestingly some directors and professionals who were the jury group of the scientific film festival, which was the next program in the que.

Thinface Ambassador Myles Rooney in Milan

“la Notte dei Ricercatori” (The researcher’s night). One day event in which all technical Universities of Milan organized public workshops with the aim to give the public a first hand experience of research in technology. As part of the event the Department of Materials Science of the University of Milano-Bicocca organized a stand with the title “It is a kind of magic. All the wonders of smart materials”. During the various activities, researches from

the department gave demonstrations of light guiding, light to electrical power conversion, electrochemistry and photochemistry. Myles was involved all the time, discussing his own work within the thinface network with the (surprisingly large number) English speaking attendees. He was particular active in exchanging information and experiences with fellow PhD students from other universities.

"**Innovation pub".** A networking event organized monthly by the University of Milano-Bicocca and intended to connect people with ideas and possible investors. Every night a few speakers having experience in tech transfer from its various points of views were asked to share their experience with PhDs and Post Docs of UNIMIB. Myles participated in such events, as the only MC fellow, discussing his project as well as career plans with other Bicocca students. Several of them decide to apply for a fellowship within HORIZON 2020.

Luca Beverina

Open Access Publications

In Horizon 2020 projects Open Access Publications will be mandatory. To emphasize it this is not the case for our Thinface ITN. But as we seek new applications we should all be aware of this fact.
Open Access means the practice of providing on-line access to scientific information that is free of charge to the end-user. This means if a researcher decides to publish an article in a journal he or she will have to make sure that it will be available open access.
Normally this will be an open access publisher ('Gold' open access) and the costs will be shifted away from the reader to the research institution or the funding institution supporting the research. Costs are eligible in H2020. Another way of open access publication ('Green' open access) will be self-archiving, where researchers can deposit the final peer-reviewed manuscript in an online archive of their choice. Institutional, subject-based and centralized repositories are accepted.
Libraries can usually assist finding the right way to open access. DOAJ offers a dictionary of open access journals and DOAB a list of open access book publishers. There are sometimes funding possibilities at the libraries too, to cover costs of open access.
Try to contact your local library for more information.
Katharina Rubahn

Events

12th International Symposium on Functional π-Electron Systems
July 19-24, 2015, Seattle, USA, Website

Smart Materials and Structures, 5th International Workshop, including a Thinface workshop
September 9-12, 2015, Marrakech, Morocco, Website

7th SCHOOL ON ORGANIC ELECTRONICS from Semiconductor to Biomolecular Interfaces / Thinface Summer School

September 14-18, 2015, Como, Italy, Website

PCAM Meeting and Thinface Mangement Meeting
September 18, 2015, Como, Italy