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Nr.11

One network event just passed, the workshop in Poland, the next one comes close: Summer School in San Sebastian which is organized by CIC NanoGUNE. The registration is still open until Mai 31.

And our first ESR has handed in her thesis!

Enjoy reading.

Yours,

Katharina Rubahn

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Scientific Breakthrough

Formation of porous silicon on silicon microcantilevers

The role of PSi on the silicon microcantilevers has been emphasized for the development of nanomechanical interfaces as biosensors. The new bimodal mechanical-optoplasmonic system for biosensing was demonstrated performing a sandwich assay for the detection of a Prostate Specific Antigen (PSA).

[Read more](#)



Scientific Breakthrough

Molybdenum-oxide hole transport layers for organic electronics

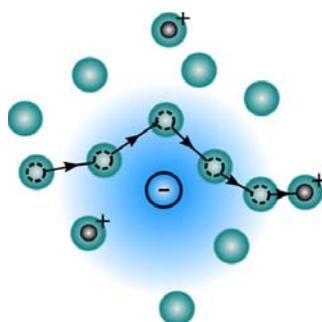
At SDU NanoSYD, University of Southern Denmark, reactive sputtering of Molybdenum oxide thin-films are conducted in order to develop metal-oxide films with tunable opto-electronic properties.

[Read more](#)



Scientific Breakthrough

Micellar coupling enables the synthesis of organic semiconductors in water, at room



temperature and under standard oxygenated atmosphere

Researchers at the University of Milano Bicocca optimized a protocol for the synthesis of different classes of both molecular and polymeric organic semiconductors enabling the use of water as the sole solvent.

[Read more](#)

Scientific Breakthrough

Fabrication of 2D Colloidal Crystals over Large Areas for Biosensing

This is the title of the first Thesis within the Thinface network that was handed in by Paola Pellacani. Apart from becoming mother in December last year she also managed another big step in her life. Her defense will be on June 23rd in Madrid. Congratulations!

Award: Horst-Günter Rubahn receives Danish 'Fyens Stiftstidende's' Researcher Prize

[Read more](#)

PCAM/Thinface Workshop in Cracow - Faculty of Physics, Astronomy and Applied Computer Science

[Advanced topics in physics and materials engineering: PCAM in Cracow 18-19 May 2017.](#)

It was a very fruitful meeting in Krakow, foreseeing new collaborations between Jagiellonian University (UJ) and SDU-MCI, as well as UJ and entire PCAM network.

[Read more](#)

Bernhard Nell presents Thinface results at international conferences in France, Germany and USA

Bernhard Nell will present results from the Thinface project at the Spring meeting of the European Materials Research Society held



between May 22 – 26. He will talk about the characterization of doped organic semiconductors using thermoelectric measurements.

Antons secondment in Sønderborg

Abhilashs secondment at Graphenea in San Sebastian

Recent publications:

31. Work Function Mapping of MoO_x Thin-Films for Application in Electronic Devices, A. L. F.

Cauduro, R. dos Reis, G. Chen, A. K. Schmid, H.-G. Rubahn and M. Madsen, *Ultramicroscopy* (2017)
DOI: 10.1016/j.ultramic.2017.03.025

30. Origin and whereabouts of recombination in perovskite solar cells, Contreras-Bernal, M. Salado, A. Todinova, L. Calio, S. Ahmad, J. Idígoras and J. A. Anta, *Phys. Chem. C*, 2017

DOI: 10.1021/acs.jpcc.7b01206.

29. Impact of Moisture on efficiency-determining electronic processes in perovskite solar cells, Salado, L. Contreras-

Bernal, L. Calio, A. Todinova, C. López, S. Ahmad, A. Borrás, J. Idígoras, J. A. Anta, *Journal of Materials Chemistry A* (2017)
DOI: 10.1039/C7TA02264F

28. Efficient and Controllable Vapor to Solid doping of the Polythiophene P3HT by Low Temperature Vapor Phase Infiltration, Weike Wang, Chaoqiu

Chen, Christopher Tollan, Fan Yang, Yong Qin, and Mato Knez. *Journal of Materials Chemistry C*, 2017.
DOI: 10.1039/C6TC05544C

[Get an overview on all publications.](#)

EU Calls of interest

MSCA ITN

Call is expected to open in autumn and closes probably in January 2018



[MSCA Individual Fellowships](#), Call opened April 11, 2017 and Closes September 14, 2017

Events

June 20-23, 2017 [Thinface/PCAM Summer school](#) on 'Surfaces and Interfaces' in San Sebastian, registration still open until 31.May.
July 10-13, 2017 Interface Properties in Organic Electronics (IPOE 2017) in Cergy-Pontoise, France

[IPOE-2017](#) will be entirely devoted to the physical phenomena occurring at organic/organic, organic/inorganic and organic/metallic interfaces, as motivated by their essential role in many (bio-)physico-chemical processes, ranging from solar energy conversion to biosensing.

More information and all events on our [webpage](#).

Antons Secondment in Sønderborg

For my secondment within the THINFACE framework I was invited to join the group of Prof. Morten Madsen from November 2016 to February 17 at the Mads Clausen Institute in Sønderborg, Denmark. I was very warmly welcomed by Morten and his group of PhDs and Postdocs. I worked closely with "future doctor" Bhushan Patil and I learned a lot about organic solar cells. As a start point, we grew and characterized several OSC focusing on the role different thickness layers and specifically a BCP interlayer that improved the performance of the solar cell. This was a very pleasant procedure, especially compared to my previous experience in depositing organic molecules. The brand-new Cryofox device worked simply perfect. The knowledge and experience of the team with the machine was so great that I encountered not a single problem when growing my devices.

To expand our knowledge of the role of the BCP layer, we investigated the performance of C70-based electron-only devices. By performing a current-voltage analysis of the electron only devices we could achieve an optimal BCP thickness. This knowledge is helping to raise the efficiency of the organic solar cells because the introduction of a BCP interlayer besides the contact is improving the electron extraction by blocking holes and avoiding recombination.

Overall it was a great secondment in a very beautiful city which I am looking forward to visit again, but next time in summer (I've never felt that cold before)



Abhilashs Secondment at Graphenea

I spent two months in the beautiful city of Donostia (San Sebastian) working with the Graphenea team as part of my secondments. My work was to develop theoretical models using density functional theory to assess the probable structure of graphene oxide. Graphene oxide flakes are usually constituted of peroxide (=O), -OH and -COOH groups. Graphene oxide structure has been studied experimentally but one of the challenges here was to distinguish the two oxygen species and assignments were made without reaching consensus [1,2]. We started by studying the adsorption energies of the fully oxidized graphene oxide structure and found that peroxide groups asymmetrically adsorbed on graphene was the most stable and in agreement with previously

studied theoretical models[1]. We went further by introducing the additional -OH and -COOH groups (for the fully oxidized case) in all the combinations available (symmetric and asymmetric adsorption sites were also covered). We found that the most stable structure for the fully oxidized case was when one peroxide group and two -OH groups were asymmetrically adsorbed as shown in Figure 1. We also studied the effect of adsorption concentration on the stability of the system. We computed the adsorption energies of the system for 50%, 25% and 12.5% coverage values and found that graphene oxide is the most stable when it is fully oxidized (50% coverage).

[1] Phys. Rev. B 79, 125435, 2007

[2] J. Phys. Chem. B, 2006, 110 (45), pp 22328–22338

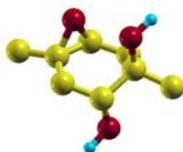


Figure 1: The relaxed structure of fully oxidized graphene oxide with one peroxide and two -OH groups asymmetrically adsorbed. The yellow atoms are carbon, red are oxygen and blue hydrogen.

Bernhard Nell presents Thinface results at international conferences in France, Germany and USA

Doping of organic small molecule semiconductors played a key role in improving the performance of organic opto-electronic devices. Using fluorinated fullerene dopants with a different degree of fluorination in various amorphous matrix materials his work relates the thin-film conductivity and thermoelectric properties to the energy level offset between matrix and dopant. Combining thermo-electric measurements with statistical models and Kinetic Monte Carlo simulations, the influence of Coulomb interactions between charge carriers and ionized dopants is revealed, explaining the low amount of mobile charge carriers generated at low doping concentrations. Moreover, new dopants leading to higher conductivities were identified, leading to better electrical contacts for more efficient organic light emitting diodes and solar cells.

Previously, part of the work was presented at the Fall Meeting of the Materials Research Society 2016 in Boston and at the Spring Meeting of the Deutsche Physikalische Gesellschaft in Dresden 2017. The dopants used in this work were provided by the Strauss-Boltalina Group of Colorado State University. The code for Kinetic Monte Carlo Simulations was developed by Markus Krammer of Thinface partner Graz University of Technology and was adapted during Bernhards secondment from July to October 2016, together with Karin Zojer. Currently Bernhard is in Graz for a second 3 month secondment.

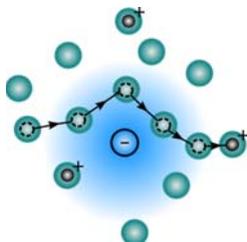


Fig. 1: A schematic representation of a molecular p-type dopant (blue), surrounded by organic semiconducting molecules (cyan). The dopant introduces a positive charge on the organic semiconductor, hereby increasing its conductivity. The negative charge left behind on the dopant forms a Coulomb potential well, which the positive charges need to overcome to actively contribute to the conductivity.



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