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Nr.7

Welcome to our 7th Thinface Newsletter which is also meant to be for the PCAM network. Since the last Newsletter we have about 10 new publications and the group at Abengoa Research contributed a patent. Read more about this and a new blog that they started at Abengoa in this Newsletter.

Yours,  
Katharina Rubahn



### Scientific Breakthrough

#### Organic Hole Transport Materials Containing an Ionic Liquid

Shahzada Ahmad, Samrana Kazim,  
Laura Calio, Manual Salado,  
Patent Application No. P201630446,  
Filed April, 2016

We have developed an hydrophobic  
doping for organic semiconductors  
to increase the charge mobilities.



### Workshop on lifetime and stability of hybrid and organic devices

Read a very interesting [report here](#).



### APS March meeting – Baltimore 2016

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**Abhilash on his secondment in San Sebastian.**



**Mina on her secondment in Madrid.**



**Read about a publication of Abhilash:** Femtomagnetism in graphene induced by core level excitation of organic adsorbates.

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



**New Blog:** Our partner Abengoa Research has established a new blog on the 'Energy of Change', followed by over 17K people on twitter and more than 7K on facebook.

Blog :

<http://www.theenergyofchange.com/>

On this blog, an article about "Thinface" appeared. [Read it here.](#)



**PhD positions and Postdoc positions are available at the University Autónoma de Madrid and at the Universtity Milano Bicocca**

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### EU-Calls of interest

[MSCA-ITN](#), Call opens September 15, 2016 and Closes January 10, 2017

[MSCA Cofund](#), Call opens April 5, 2017 and Closes September 28, 2017



Two Thinface events are ready for registration: a summer school on 'Organic Electronics' in July and a workshop on Dynamical Phenomena at Surfaces (WDPS-17) in Milan and many more events in the field.

[Read more](#)

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## Breaking News: Patent on Organic Hole Transport Materials Containing an Ionic Liquid

A thin layer of p-type (hole transporter) material is used for the fabrication of sensitized solar cells (dye or perovskite solar cells) to extract holes efficiently and transport them back to the electrode. Since the existing hole transport materials do not show the required charge mobility for solar cell applications, it is further doped with ionic salts. Most of the ionic salts are highly hygroscopic and the increase in charge mobility is achieved at the cost of device stability. We have developed a hydrophobic dopant which increases the device performance, without effecting the device stability.

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**Prof. Gian Paolo Brivio, Dr. Daniel Sánchez-Portal, Moritz Müller, and Abhilash Ravikumar**

## **APS March meeting – Baltimore 2016 (by Abhilash and Moritz)**

According to the American Physical Society (APS), this year's March meeting was one of their biggest March meetings to date, with 9,874 attendees and 8,985 abstracts. Four of the contributions came from members of the initial training network Thinface. We were very happy to have had the chance to visit this enormous event together with our supervisors Prof. Gian Paolo Brivio and Dr. Daniel Sánchez-Portal. The conference covered a broad range of experimental as well as theoretical works with highly specialized sessions devoted to topics such as soft matter physics, superconductivity, quantum information, and photovoltaic applications. We had the opportunity to listen to Nobel laureates as well as to join more general discussions on the peer review process. For us two PhD students from the training network it was exciting to attend the talks from the total number of six sessions on “Advances in Density Functional Theory” and to actually meet some of the heroes of the field we are working in. The amount of sessions devoted to this theory underlines its role

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as the current work horse of modern electronic structure calculations.

We also had the opportunity to present our results in front of an international audience of scientists and to see the work presented by other PhD students from all over the world. Abhilash reported his results on “Femtomagnetism in graphene induced by core-level excitation of organic adsorbates” and Moritz presented his current work about the “Influence of structural fluctuations on lifetimes of adsorbate states at hybrid organic-semiconductor interfaces”.

Our attendance of the conference really allowed us to place our work in the context of what is currently done, to take a glimpse at the first and foremost frontiers within the field of our work, to meet new people, and to participate in discussions. In that sense the attendance of the event has been a great experience for us and was a good practice for presenting our work in front of an expert audience. Maybe there is a chance to visit next year's March meeting. The venue will be located in the awesome city of New Orleans.

Take a look at other attendees' highlights of this years conference at [www.youtube.com/watch?time\\_continue=1&v=0SadJ9GGZO8](http://www.youtube.com/watch?time_continue=1&v=0SadJ9GGZO8)

This link can also be found on the APS web page [www.aps.org/meetings/march](http://www.aps.org/meetings/march)

Cheers,  
Abhilash and Moritz

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## Abhilash on his secondment in San Sebastian



My secondments took place in the beautiful Basque city of San Sebastian, which is a coast in the north of Spain bordering France. I worked at the Center of Material Physics (CFM) under the guidance of Dr. Daniel Sanchez Portal.

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of core excited organic molecules adsorbed on graphene/nickel (111) system. We perform Density Functional Theory calculations coupled with non equilibrium Greens function techniques to evaluate this charge transfer lifetimes. Even though graphene on nickel systems have been extensively studied, setting up these calculations with molecules adsorbed on them significantly increase the system size and this was a major challenge requiring large computational resources. Fortunately with the help of the state of the art clusters and large computational facilities available here at CFM and DIPC (Donostia International Physics Center) this was accomplished. We have now studied the ground state properties of this system and have begun looking at the nitrogen 1s core excited case. These results will be compared to the experimental results performed using the core hole clock technique. Due to the asymmetric distribution of states in Nickel for different spin channels, one could expect different charge transfer lifetimes for the two spin channels which would be very interesting.

During my stay here I also had the opportunity to participate in the APS – March meet where I presented a talk on my previous work- “Femtomagnetism in graphene induced by core level excitation of organic adsorbates”. This work has also been recently published in Nature - Scientific Reports (Ravikumar, A. et. al. Sci. Rep. 6, 24603). The conference was a very lively affair with a melting pot of physicists from all over the world. In particular was a talk given by Nobel laureate Dr. Steven Weinberg on his recent book “To explain the world-The Discovery of Modern Science” which was very interesting. We also had talks from Prof. Brivio, Dr. Sanchez Portal and Moritz Muller from our THINFACE community about their research which was very informative.

## **Mina on her secondment in Madrid**

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I stayed at Universidad Autónoma de Madrid from Oct 1st -Nov.17th 2015.

Working at the UAM under the supervision of Miguel Manso was a great experience. My work was focused on the investigation of large-area periodic gold nano-triangle arrays, which are prepared from Langmuir-Blodgett film, using a lithographic method based on selfassembly of polystyrene/silica nano-spheres. The main purpose of this work was to manipulate the plasmonic response of targeted substrate by using different size of periodic gold nano-triangles to obtain the optical absorption enhancement in organic solar cells. In this work, I studied the different size of triangular shaped nanoparticles in the hexagonal array, through changing the mask morphology by temperature processing and varying the size of nanoparticles.

The visit engaged my interest in nanostructure fabrication and strengthened my experience by working in the different scientific area. In addition, the secondment gave me the opportunity to gain a new perspective about working in a different laboratory and overcome the challenges of the new environment.

The outcome and result of my work is accepted for poster presentation at the International Conference on Hybrid and Organic Photovoltaics (HOPV16).

Of course, my report would not be complete without mentioning where and how I spent my free time! My most memorable adventures I had going to the pottery class. An honorable mention goes out to the Madrid attractions such as Buen Retiro Park, Royal place, Mercado de San Miguel and churros with chocolate!

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## **Femtomagnetism in graphene induced by core level excitation of organic adsorbates**

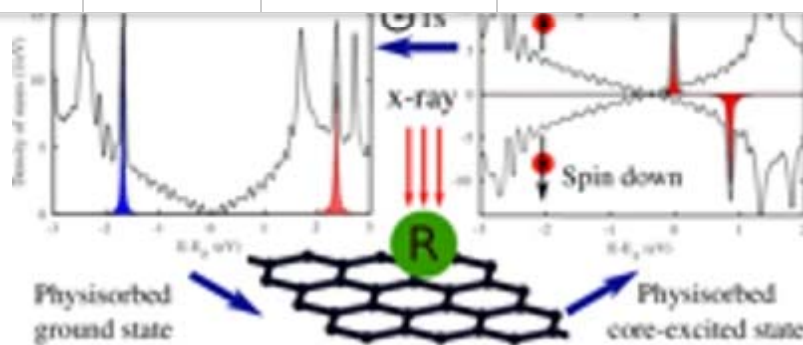
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We predict the induction or suppression of magnetism in the valence shell of physisorbed and chemisorbed organic molecules on graphene occurring on the femtosecond time scale as a result of core level excitations [1]. For physisorbed molecules, where the interaction with graphene is dominated by van der Waals forces

and the system is non-magnetic in the ground state, numerical simulations based on density functional theory show that the valence electrons relax towards a spin polarized configuration upon excitation of a core-level electron. The system is magnetic until the core electron de-excites via one of the several electronic decay channels [2,3]. The magnetism depends on efficient electron transfer from graphene on the femtosecond time scale. On the other hand, when graphene is covalently functionalized, the system is magnetic in the ground state showing two spin dependent mid gap states localized around the adsorption site [4]. At variance with the physisorbed case upon core-level excitation, the LUMO of the molecule and the mid gap states of graphene hybridize and the relaxed valence shell is not magnetic anymore.

#### References

- [1] Ravikumar, A. et al. Femtomagnetism in graphene induced by core level excitation of organic adsorbates. *Sci. Rep.* 6, 24603; doi: 10.1038/srep24603 (2016).
- [2] Adak, O. et al. Ultrafast Bidirectional Charge Transport and Electron Decoherence at Molecule/Surface Interfaces: A Comparison of Gold, Graphene, and Graphene Nanoribbon Surfaces. *Nano Letters* 15, 8316–8321 (2015).
- [3] Fratesi, G., Motta, C., Trioni, M. I., Brivio, G. P. & Sánchez-Portal, D. Resonant Lifetime of Core-Excited Organic Adsorbates from First Principles. *The Journal of Physical Chemistry C* 118, 8775–8782 (2014).
- [4] Santos, E. J. G., Ayuela, A. & Sánchez-Portal, D. Universal magnetic properties of sp<sup>3</sup>-type defects in covalently functionalized graphene. *New Journal of Physics* 14, 043022 (2012).



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## PhD positions and Postdoc positions are available at the University Autónoma de Madrid and at the University Milano Bicocca

**Universidad Autónoma de Madrid (UAM)**, Spain, is looking for a PhD od PostDoc position in Physics and Chemistry of Advanced Materials. UAM is launching a call for PhD and Post Doctoral positions in a wide range of subjects. If you have a reference contact at UAM contact them. For further details on participating groups or topics contact: miguel.manso@uam.es.

Deadline for PhD applications: June 28, 2016. The call is open to valuable candidates from all over the world.

PostDoc positions shall comply with Marie Curie mobility rule and have no final closing date at the moment (foreseen mid july 2016).

A whole set of different PHD and Postdoc positions in different fields is offered at the **University of Milano Bicocca** in Italy. Find the [announcements here](#). For positions in Material Sciences and Nanotechnology go to page 23 in the document.



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