THINFACE
European Training Network

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Welcome to our Newsletter 2

The Network lives from its enthusiastic students

It's a pleasure to me to present a few nice photographs from a very good Winter School. The participating students loved it so much that all of them would recommend it to others! I think this truely is an honour for the organizers and all that contributed to this success.

If someone would like to communicate with these wonderful students and discuss science with them try out our Thinface

Group on LinkedIn.

This newsletter introduces some new instruments like the Orion Microscope and a PVD Cluster system, that are available for external use. I look forward to receive some more interesting news on new instrumentation and to the experiences on first secondments.

Also this time three projects are introduced.

Have a great time reading!
Katharina Rubahn

In this issue

Mme Curie in Snow as seen during the Winter School in Miraflores de la Sierra.

Winter School 2015

Some words from a student.

This Winter School took place in Miraflores de la Sierra, a quiet village in the mountains nearby Madrid. The definition “winter” was totally justified since we had snow (and then a really nice panorama) all the week! This school has been a

good opportunity for all the ITN students to meet after the previous experience in Sønderborg and there has been time to discuss, formally and informally, about progress, doubts and future plans, as well as to have fun together.
The school programme covered a wide range of topics on soft skills and presented us several interesting perspectives from an academic and an industrial point of view. Most of the talks were structured in an interactive way, motivating the students to actively participate and helping to focus on their needs. Some of them were focused on suggestions about the organization of our PhD work and some others were useful to start thinking about a smart way to tailor our professional career. In particular, the personal experience of some lecturers, reporting both problems and success, has been valuable for a better understanding of the topic discussed in a real contest. I had a very positive impression from this school, many interesting hints to think about!

Paola Pellacani

The THINFACE winter school was hosted in a very comfortable Residence of the Autonoma University in a somewhat secluded place, surrounded by pine trees, in the Sierra. The isolated atmosphere was enhanced by snow blizzards and the very cold temperature outside which lasted for the full time of the school. I do not know whether this situation may have favored the interaction among lecturers and students or not. I was the only senior scientist who stayed also overnight for the full period of the school and participated in all lectures also giving one on *Career, CV and Networking.* I enjoyed the program certainly more extended

than that at similar courses on soft skills at most Universities. With about 28 hours of lectures, this school was able to cover the various topics in depth. The presence of speakers from various companies (Abengoa, McWinnies, Boeing, Plasmore and Pirelli), managers and entrepreneurs, could help the students to get a wider perspective for their future.
I also had the opportunity to meet all students, most of them from THINFACE, but also from PCAM partner Universities not involved in this ITN project. All of them looked eager and concerned to take advantage of this opportunity and considered it very useful to help choosing their activity after the Ph.D. At dinner and after it I was often the only scientist staying at the Residence and mixed with students, but I get the feeling that they could have liked more senior people to be there and informally exchange ideas with them. Anyway I got the impression that the world future, technological, cultural and social, is of importance to the young people, especially for ITN students who, in the next decades, may have responsibilities in our so fast developing and changing planet. Why not a THINFACE school on this topic?
Finally I wish to point out the perfect organization of Prof. Miguel Manso, who was also able to offer us a trip to a nearby castle in a chill weather and the magic of a nice illusionist.

Gian Paolo Brivio.

ny name is Moritz Müller
am a 26 years old
icist from Munich in
many. I studied at the
nical University of Munich
M) and Denmarks
nical University in
enhagen specializing in
neering physics during my
ter's studies. My main
ests are electronic
ture calculations with
cations in
Nanotechnology.
This involves computational modeling of surface mounted structures such as the description of self assembled

free-base porphine layers on coinage metal surfaces in my master's thesis (Group of Prof. Dr. Karsten Reuter, Technische Universität München). Since mid of May 2014 I work for CIC nanoGUNE and I am located at the “Centro de Física de Materiales” (CFM) in Donostia – San Sebastián, Spain. As a member of the group of Dr. Daniel Sanchez-Portal I am investigating the lifetimes of HOMO and LUMO states of organic molecules adsorbed on TiO2 surfaces relevant for applications in photovoltaics.

Besides doing physics I like swimming and running and I enjoy listening to Jazz, classical and rap music. I am looking forward to seeing all of you at the next summer school at Lake Como. Please do not hesitate to contact me.

am Abhilash Ravikumar, Bangalore, India. I uated from Amrita School gineering in Electronics Communication neering. I did my post uation in Nanotechnology National Institute of nology, Karnataka, thkal and my research s was on “Molecular Dynamics simulations of stable orientations of graphene on Silicon (001) substrate” at the Aerospace Department, Indian Institute of Science, Bangalore, India. My research interests are electronic structure calculations with applications in nano-

electronics and device mechanics. I am currently doing my Ph.D at University of Milano, Bicocca, Milano, Italy under the guidance of Dr. Gian Paolo Brivio. I am investigating the effect of adsorption of organic molecules on graphene. I am interested at looking at the electronic properties of these systems, their excited state charge transfer lifetimes and computational spectroscopy.

I love playing cricket and basketball. I enjoy painting, reading novels, writing poems and travelling. Please feel free to contact me if you share my interests.

Get insight into Moritz project:

Developing a method to compute charge-transfer times in organic photovoltaic systems

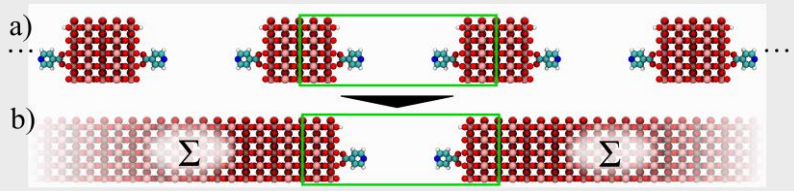


Fig. 1: *Organic adsorbate (isonicotinic acid) at the rutile surface TiO_2(110), schematic depicting different computational approaches: Periodic slab approach within the DFT code Siesta (a), and coupling of the central region (green box) to semi-infinite electrodes within the Greens function code Transiesta.*

Dye-sensitized solar cells and related organic photovoltaic devices are considered to be promising candidates for future energy devices. Nonetheless, the underlying processes governing charge transfer at semiconductor interfaces in such devices are by no means fully understood. Modeling approaches describing the physics behind the fundamental electron dynamics in such systems and in particular the physics of excited states push currently available techniques to the limits of their capabilities. We strive for a better comprehension of organic solar cells comprising rutile (TiO_2) substrates on the basis of computer modeling. Our goal is to achieve a detailed understanding of the charge transfer process by employing state of the art Greens function techniques on top of density functional theory (DFT) calculations.

These transfer processes can be illustrated in the following quantum mechanical picture: An initial wave-packet localized on a dye molecule at the TiO_2 surface describes an electron residing on the adsorbate after its precedent excitation due to light radiation. This electron decays with a certain probability into the substrate which characterizes the lifetime of the excited electron. In the wave picture this is the time

until the localized wave-packet delocalizes into the substrate – a process on the time scale of a few femtoseconds.
In our approach [1,2] we start investigating these lifetimes by calculating the ground state electronic structure of the system in a classical slab approach [Fig. 1 a)] employing periodic boundary conditions in the DFT code Siesta. The computational unit-cell (green box) is repeated periodically in all three dimensions of space. In Fig. 1 a) only repetitions in the direction perpendicular to the surface are shown and subsequent slabs are separated by vacuum regions. This procedure allows only for a few atomic layers of the substrate to be computationally feasible. We employ the transport code Transiesta in order to effectively model the coupling of a central region to fully semi infinite electrodes [Fig. 1 b)]. Therein mathematically the system is described by a Greens function which yields the response of the central unit (green box) to the semi-infinite substrate by incorporating the self-energies (Σ) of the latter into an effective Hamiltonian.
We finally obtain the lifetimes of excited electrons by explicitly projecting the Greens function of the full substrate system onto the initial wave packets. The imaginary part of the latter projections results in a projected density of states (PDOS) from which we extract the lifetimes by measuring the width of resonance peaks therein.
We have been able to test the above scheme after successfully implementing the projection into a current development version of the Greens function code Transiesta. This implementation allows us to tackle larger systems and to stay in close vicinity to the ongoing code development. The implementation has so far been tested on systems concerning core excited Argon atoms adsorbed on

metal surfaces. The results of our spin polarized calculations state that majority excited electrons on Ar are longer-lived than minority excited electrons on Ar. This is in agreement with experiments [3] and emphasizes the potential of the technique to be applied to large organic molecules on TiO_2 substrates.

[1] G. Fratesi, *et al.*, J. Phys. Chem. C **118**, 8775–8782 (2014)
[2] D. Sánchez-Portal, Prog. Surf. Sci. **82**, 313–335 (2007)
[3] F. Blobner, *et al.*, Phys. Rev. Lett. **112**, 086801 (2014)

Get insight into Abhilashs project:

Adsorption of organic molecules on graphene

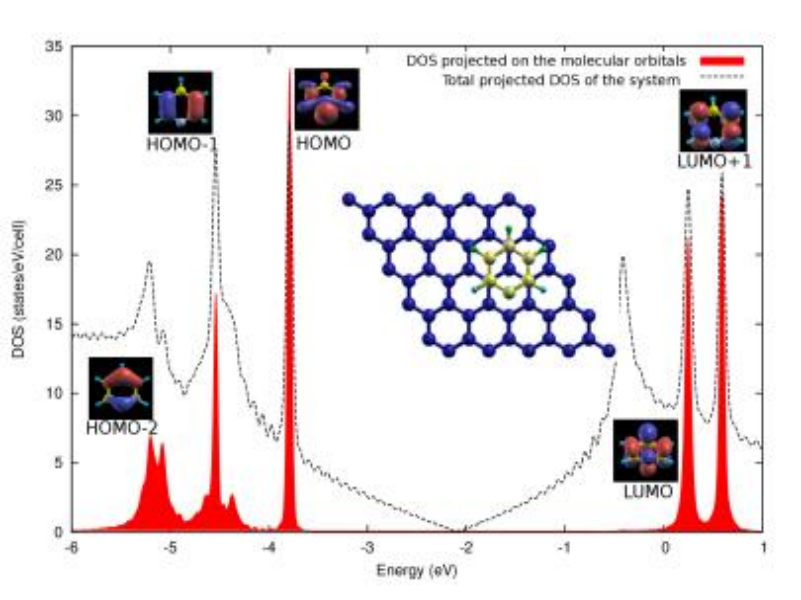


Figure1: The density of states of pyridine adsorbed graphene and the density of states projected on the molecular orbitals (red), arranged from HOMO-2 to LUMO+1. Inset shows the molecular orbitals of pyridine in gas phase.

Graphene is a two dimensional crystalline allotrope of carbon with honeycomb lattice structure and has been extensively studied since its discovery in 2004 since it displays several unique properties. Graphene and its composites have various potential applications such as efficient gas sensors, novel spintronic devices and transparent electrodes for photovoltaics.

Our study deals with understanding the interaction of organic adsorbates on graphene such as Pyridine, (C_5H_5N) and 4, 4'-bipyridine, $(C_5H_5N)_2$. The stable adsorption configurations of these molecules are determined by density functional theory considering van der Waals correction, taking into account the translational as well as rotational degrees of freedom of the molecule. Pyridine placed parallel to the graphene sheet, with its nitrogen atom at the center of the graphene ring is found to be the most stable configuration, with an adsorption energy of -0.60 eV in agreement with results in the literature [1]. In gas phase, 4,4'-bipyridine has a

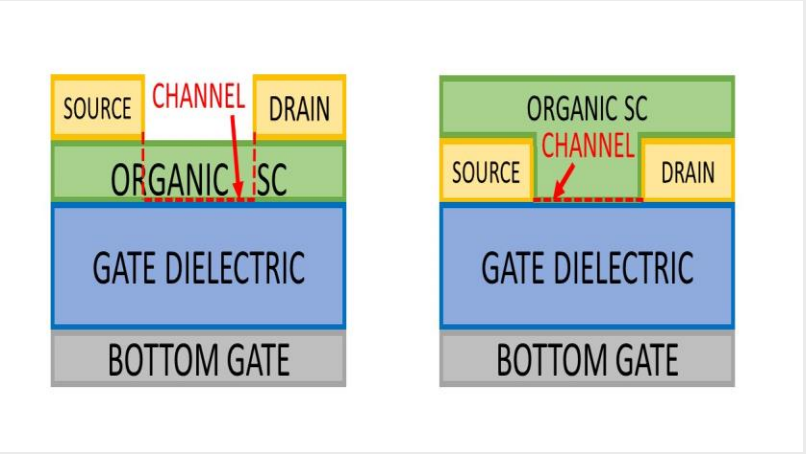
torsional angle of 33° which reduces significantly (to about 19°) when placed on graphene. The stable configuration is when the pyridyl rings of the molecule follow a similar stacking as found in graphite.

The electronic band structure and the density of states of pyridine adsorbed on graphene reveals little interaction of the molecule with the substrate. The spatial overlap of the molecular orbitals with the substrate bands induces an energy broadening of their features in the density of states as seen in Figure 1. Such width can be related to the electron transfer times at the molecule/graphene interface which is in the order of few femtoseconds to a few hundred femtoseconds for different orbitals. However for a more appropriate estimate of such lifetimes, we would like to determine the core-hole excited density of states and calculate near-edge X-ray absorption fine structure (NEXAFS) spectrum of the system using the transition-potential approach [2, 3]. The effect of a metal substrate supporting graphene will eventually be studied by considering these organic molecules adsorbed on graphene placed on nickel (111). Future plans also include working at Centro de Física de Materiales (CFM), CIC nanoGUNE, in Donostia – San Sebastián, Spain to examine phonon effects on the lifetime with Dr. Daniel Sanchez-Portal.

[1] E.N. Voloshina, et al., Chem. Phys. Lett.10 (2011) 220-223

[2] L. Triguero, et al., Phys. Rev. B, 58(1988), P8097

[3] G. Fratesi, et al., J. Phys. Chem. C 117 (2013) 6632-6638



a)Staggered Architecture: Top-contact Bottom-Gate b)Coplanar Architecture: Bottom-contact Bottom-gate

The main difference between organic and inorganic transistors is that in organic transistors the transport takes place through hopping between molecular orbitals instead of electronic bands[1]. Drift-diffusion is a simulation method that is widely used to simulate the performance of inorganic transistors. Fortunately we can also use it for organic semiconductors despite this difference in the carrier transport[2]. Using a self-consistent drift-diffusion technique we analyze the general performance of transistors while modifying several parameters such as channel length, organic and dielectric thicknesses or applied voltages.

By analyzing local charge carrier densities and potentials, we were able to study the contact resistances in the metal-OSC interface. We found out that injection processes are substantially different for Staggered (Fig.1a) and for Coplanar (Fig.1b) OTFTs.

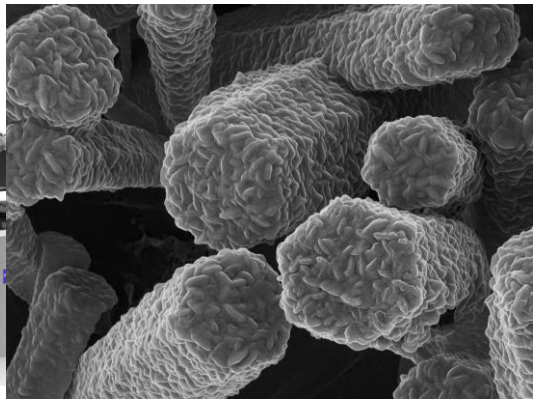
There are two mechanisms that lower the injected current in a top-contact OTFT: The energetic difference between the Fermi energy level of the metal and the transport level at the organic semiconductor act as a potential barrier that reduces injection efficiency. Moreover, there is under contact an extra low conductance region that carriers need to go through. Being transmittance through this bulk region low, current will go through a high resistance path. This so called access resistance [3] will be bigger as the OSC layer gets thicker.

In bottom-contact there is no access resistance, but increasing the dielectric thickness will decrease the potentials in the contact/OSC interface, resulting into a smaller barrier reshaping. For the same operation point of OTFTs we find an ON state for small dielectric thickness and an OFF state for thicker dielectrics. This results into an increment of the threshold voltage on the transfer curve. Results of this research are going to be published soon.

After finding this, we focused into short channel effects[4]. Our approach is to aggressively reduce the length of the channel. By now we are able to observe that

the linear regime vanishes as we get close to 500nm.
Unfortunately, our current method doesn't allow us to deal with channel lengths in the 100nm range. For very strong fields all three equations (drift, diffusion and Poisson) become very coupled, and they cannot be solved independently anymore. At this point our approach might be to switch from Scharffeter-Gummel to a Gummel block iteration technique[5]. This algorithm allows us to solve all equations (drift, diffusion and poison) iteratively but without time-dependence. We are confident that this new method will be able to handle better strong fields.

[1] G.Horowitz, Organic Field-Effect Transistors, Adv. Mater. 1998, 10, No.5, 365-377 (1999)
[2] W.Tress et. al., Influence of Hole-Transport Layers and Donor Materials on Open-Circuit Voltage and Shape of I-V Curves of Organic Solar Cells, Adv. Mater. 2011, 21, No.11, 2140-2149 (2011)
[3] M. Gruber et al., Relation between injection barrier and contact resistance in top-contact organic thin-film transistors, Organic Electronics 13, 1887–1899 (2012)
[4] J. N. Haddock et. al., A comprehensive study of short channel effects in organic field-effect transistors, Organic Electronics 7, 45-54 (2006)
[5] Can E. Korman et. al., A globally convergent algorithm for the solution of the steady-state semiconductor device equations, J. Appl. Phys. 68, 1324-1334 (1990)



Orion- He-Ion microscope at SDU in Sønderborg

An instrument that combines advantages of scanning and transmission electron microscopes and can be used by multiple users.

I am glad to give you a short announcement of our new facilities, Orion NanoFab ion microscope that has been very recently installed at MCI SDU.
The Orion technology comprises the new achievements in the areas of high-resolution-imaging and nano-fabrication.
The first device was marketed in 2006 and there are only about 30 instruments installed at the moment. Our instrument is the first and so far the only one of this kind in Scandinavia
The heart of Orion microscope is the so-called field-ion-source that emits atomically sharp beams of either Helium or Neon ions capable of generating both high-resolution images and nanostructures
The main advantages of the Orion microscope include: superior resolution, atomic layer sensitivity, no charging artefacts, high focus depth and many others.
Orion is capable of fabricating features with dimensions ranging from several micrometers to few nanometers.
The nanostructures can be both cut away and deposited with an especial gas injection system.
Some of the charachteristics in brief:

	TEM (120 kV)	**ORION**
Source	Tungsten or LaB6	GFIS Gas Field Ion Source
Imaging	Transmission	Surface with large depth of focus
Resolution	0.34 nm < 1.5 nm (STEM)	0.35 nm
Preparation	Time consuming	'Not necessary', no charging artefacts
Sample Size	3 mm diameter	Limited by chamber size
Interpretation	Easy – expert level	Easy
Analytics	Diffraction additional: EELS, ESI, EDX	Additional: EDX, Diffraction
Nano structuring	No!	Wide range with He^-, Ne^- og Ga^-

Cryofox PVD cluster system, Polyteknik A/S

An unique cluster deposition system has recently been installed at the Mads Clausen Institute, University of Southern Denmark. The system combines three high-vacuum chambers for deposition of organic molecules (thermal), metals (thermal) and metal-oxides (reactive sputtering) through one transfer chamber with a robot arm for automatic recipe control. In addition, the transfer chamber is connected to a glovebox system for loading and unloading of samples from and to an inert atmosphere. The system is specifically designed for complete fabrication or organic solar cells and light-emitting devices in one PVD system.

For more information, please contact Morten Madsen: madsen@mci.sdu.dk

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Conferences

International Conference on Organic Electronics 2015, Erlangen, June 15-17, 2015, https://www.icoe2015.de/

Next Generation Organic Photovoltaics, June 28-July 1, 2015, Groningen, Netherlands
http://conference.groningensolar.nl/welcome

ICMAT in Singapur, June 28- July 3, 2015,
http://www.mrs.org.sg/icmat2015/public.asp?page=home.asp

12th International Symposium on Funktional π-electron Systems, July 19-24, 2015, Seattle, USA
http://depts.washington.edu/fpi12/

SPIE Optics and Photonics, August 9-13, 2015, San Diego, USA
http://spie.org/x30491.xml

Psi-K Conference in San Sebastian, September 6-10, 2015:
http://nano-bio.ehu.es/psik2015/programme.html

Thinface Summer School: 7th SCHOOL ON ORGANIC ELECTRONICS from Semiconductor to Biomolecular Interfaces
Register before April 25, 2015
http://oeri.lakecomoschool.org/

Electronic Structure and Processes at Molecular-Based Interfaces, October 14-16, 2015, http://energy.arizona.edu/education/espmi8-conference

Summer School: ECOLE SIMULATION NUMERIQUE à Jussieu (Paris 5ème) June 1-4, 2015
The summer school proposes an initial training composed of 4 half days of lecture (in french) and three half days of practicals (can be in english upon request). Topics are Monte-Carlo, molecular dynamics, ab-inition simulations, DFT, Quantum Monte Carlo, excited states
No fees apply, housing and travel cost are not covered.
Registration : philippe.depondt@insp.jussieu.fr
More information: http://www.insp.jussieu.fr/jsnum/