

WINTERSCHOOL ON ORGANIC ELECTRONICS

The Role of Interfaces

Organizers:

Egbert Zojer, Roland Resel - TU Graz and N. Koch - HU Berlin

January 26th - January 31st, 2008

Universitäts-Sportheim Plannersalm

Donnersbach, Austria



| | 01/26/2008 Saturday | 01/27/2008 Sunday | 01/28/2008 Monday | 01/29/2008 Tuesday | 01/30/2008 Wednesday | 01/31/2008 Thursday |
|-------|------------------------|---------------------------|---------------------------|---------------------------|---------------------------|---------------------------|
| 08:30 | | Ramsey | Ueno | Müllen | Rabe | Stadlober |
| 09:20 | | Bröker | Hlawacek | Beverina | Douhard | Ruderer |
| 09:40 | | Berkebile | Salzmann | | Mine | Haase |
| 10:00 | | <i>Break</i> | <i>Break</i> | 10:10 <i>Break</i> | <i>Break</i> | <i>Break</i> |
| 10:30 | | Witte | Bonfiglio | List | Zeppenfeld | Brinkmann |
| 11:20 | | Asadi | Zojer | Cristadoro | Mikhnenko | Resel |
| 11:40 | | Käfer | Cosseddu | Schiek | Bruevich | Koini |
| 12:00 | | <i>Lunch</i> | <i>Lunch</i> | <i>Lunch</i> | <i>Lunch</i> | <i>Lunch</i> |
| 13:00 | | <i>leisure activities</i> | <i>leisure activities</i> | <i>leisure activities</i> | <i>leisure activities</i> | <i>leisure activities</i> |
| 17:10 | | Heimel | Neher | Schreiber | Vázquez | Harkema |
| 18:00 | <i>Dinner</i> | <i>Dinner</i> | <i>Dinner</i> | <i>Dinner</i> | <i>Dinner</i> | <i>Dinner</i> |
| 19:00 | Welcome ! | Romaner | Jakabovic | Lex | Rangger | |
| 19:20 | | POSTERS | POSTERS | POSTERS | POSTERS | |
| 21:00 | | | | | | |

Sunday, 27th January 2008

08:30 - 10:00 Chairman: R. Resel / E. Zojer

08:30 – 09:20: M. G. Ramsey

Growth and electronic band structure of electronically active organic films

09:20 – 09:40: B. Bröker

Metal work function tuning with new molecular acceptors

09:40 – 10:00: S. Berkebile

Contact formation on organic films: A tale of three inorganics

10:00 – 10:30: Coffee break

10:30 - 12:00 Chairman: J. P. Rabe

10:30 – 11:20: G. Witte

Self-assembled monolayers

11:20 – 11:40: K. Asadi

Modifying electrodes in field-effect transistors by self-assembled monolayers

11:40 – 12:00: D. Käfer

New approach for metallization of SAMs by making use of electronegativity

12:00 – 13:00: Lunch

13:00 – 17:00: Leisure activities

17:10 - 20:00 Chairman: Harkema

17:10 – 18:00: G. Heimel

Quantum mechanical simulation of self-assembled monolayers

18:00 – 19:00: Dinner

19:00 – 19:20: L. Romaner

DFT calculations including van der Waals dispersion forces: PTCDA on Ag(111)

19:20 – 21:00: Poster session

Monday, 28th January 2008

08:30 - 10:00 Chairman: M. Brinkmann

08:30 – 09:20: N. Ueno

Advanced UPS studies of weakly interacting organic layers

09:20 – 09:40: G. Hlawacek

Zeno effect and step edge barrier in organic thin films

09:40 – 10:00: I. Salzmann

The electronic structure of Pentacene/Fullerene layered and co-deposited thin films on poly(ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT:PSS)

10:00 – 10:30: Coffee break

10:30 - 12:00 Chairman: N. Koch

10:30 – 11:20: A. Bonfiglio

Organic Field Effect Transistors

11:20 – 11:40: E. Zojer

Controlling the characteristics of organic thin film transistors through interface modifications

11:40 – 12:00: P. Cosseddu

Flexible Organic Field Effect Transistors with tunable threshold-voltage

12:00 – 13:00: Lunch

13:00 – 17:00: Leisure activities

17:10 - 20:00 Chairman: G. Witte

17:10 – 18:00: D. Neher

Organic Light-Emitting Devices and Interface Tuning

18:00 – 19:00: Dinner

19:00 – 19:20: J. Jakabovic

Preparation and properties of parylene layers for OFETs

19:20 – 21:00: Poster session

Tuesday, 29th January 2008

08:30 - 10:00 Chairman: N. Ueno

08:30 – 09:20: K. Müllen

Functional macromolecules for organic electronics

09:20 – 10:00: L. Beverina

Organic chemistry as a tool for surface modification

10:10 – 10:30 :Coffee break

10:30 - 12:00 Chairman: F. Schreiber

10:30 – 11:20: E. List

Fabrication techniques for organic electronics

11:20 – 11:40: A. Cristandoro

Soft-landing mass spectrometry of rigid p systems for ordered and ultrapure layers for organic electronics

11:40 – 12:00: M. Schiek

Nanofibers from functionalised organic semiconductors

12:00 – 13:00: Lunch

13:00 – 17:00: Leisure activities

17:10 - 20:00 Chairman: M. G. Ramsey

17:10 – 18:00: F. Schreiber

Structural characterisation of organic thin films

18:00 – 19:00: Dinner

19:00 – 19:20: A. Lex

Investigation of chemically and photochemically reactive siloxane thin layers for surface modification

19:20 – 21:00: Poster session

Wednesday, 30th January 2008

08:30 - 10:00 Chairman: H. Vázquez

08:30 – 09:20: J. P. Rabe

Scanning probe characterisation of organic layers

09:20 – 09:40: B. Douhard

Application of ToF-SIMS and XPS in organic electronics

09:40 – 10:00: N. Mine

Depth profiling polymers and multi-layers with very low energy ions

10:00 – 10:30: Coffee break

10:30 - 12:00 Chairman: A. Stadlober

10:30 – 11:20: P. Zeppenfeld

Optical characterisation of organics on surfaces

11:20 – 11:40: O. V. Mikhnenko

Low temperature study of the exciton diffusion in conjugated polymers

11:40 – 12:00: V. Bruevich

Possibilities of exohedral metalloc complexes of fullerenes for polymer solar cells

12:00 – 13:00: Lunch

13:00 – 17:00: Leisure activities

17:10 - 20:00 Chairman: D. Neher

17:10 – 18:00: H. Vázquez

Modelling Organic/Metal Interfaces

18:00 – 19:00: Dinner

19:00 – 19:20: G. Rangger

Bonding of organic acceptors on coinage metals – combining theory and experiment

19:20 – 21:00: Poster session

Thursday, 31st January 2008

08:30 - 10:00 Chairman: A. Bonfiglio

08:30 – 09:20: B. Stadlober

The role of interfaces for device degradation

09:20 – 09:40: Ruderer

Structure and Morphology of Conducting Polymerfilms for Photovoltaic Application

09:40 – 10:00: A. Haase

Organic photodiodes on printed ITO coatings for flexible organic photodiodes

10:00 – 10:30: Coffee break

10:30 - 12:00 Chairman: P. Zeppenfeld

10:30 – 11:20: M. Brinkmann

Using Transmission Electron Microscopy to analyze the structure and morphology of organic functional materials

11:20 – 11:40: R. Resel

Structural properties of sexiphenyl / pentacene / sexithiophene triple layer organic heterostructure on a Cu(110)-(2x1)O surface

11:40 – 12:00: M. Kioni

Epitaxial order of pentacene on Cu(110)-(2x1)O induced by surface corrugation

12:00 – 13:00: Lunch

13:00 – 17:00: Leisure activities

17:10 - 20:00 Chairman: K. Zojer

17:10 – 18:00: S. Harkema

Challenges for the industrial realization of organic electronics

18:00 – 19:00: Dinner

Posters

Nanostructured and highly oriented polycarbonate layers

C. Vergnat, M. Brinkmann, J.F. Legrand, C. Contal, J.C. Wittmann

Polymer thin film characterization: A combined approach by X-ray reflectivity and spectroscopic ellipsometry

H. - G. Flesch (a), O. Werzer (a), P. Frank (a), A. Blümel (a), J. Kováč (b), J. Jakabovič (b), G. Jakopic (c), R. Resel (a)

Self assembly of multicomponent nanostructures driven by hydrogen-bond

C.A. Palma (a), L. Piot (a), A. Llannes (b), D. Bonifazi (b,c), P. Samori (a,d)

Depolarization effects in self-assembled monolayers

D. Cornil, Y. Olivier, V. Geskin, J. Cornil

Localized charge transfer in a molecularly doped conducting polymer

A. Vollmer (a), Emad F. Aziz (a), S. Eisebitt(a), W. Eberhardt (a), P. Pingel (b), D. Neher (b), N.Koch (c)

Novel Copolymers as semiconducting material for OFETs and OPVs

P. Piyakulawat, A. Keawprajak, U. Asawapirom

Synthetic strategies towards large planar acceptors for organic electronics

R. Rieger

Nucleation-governed reversible self-assembly of an organic semiconductor at surfaces: Long-range mass transport forming giant functional fibers

R. C. Savane (a), G. De Luca (a), A. Liscio (a), P. Maccagnani (c), F. Nolde (d), V. Palermo (a), K. Müllen (d), P. Samori (a,b)

AFM, Ellipsometry, XPS and TEM on ultra-thin oxide/polymer nanocomposite layers in organic thin film transistors

A. Fian (a), A. Haase (a), B. Stadlober (a), G. Jakopic (a), N. B. Matsko (b), W. Grogger (b)

Packing of planar organic molecules: interplay of van der Waals and electrostatic interaction

M. El Helou (a), D. Käfer(a), C. Gemel (b), G. Witte(a)

Energy transfer in organic system of conjugated polymer and its ground-state charge transfer complex

S. Zapunidi, O. Paraschuk

Theoretical study of electron transfer in polypyrrole molecular nanowires placed between platinum electrodes

V. Rozsival, P. Jelinek

Surface modification of thin organic layers using the photo-Fries reaction

T. Hoefler (a), T. Grießler (a), G. Hernández Sosa (b), G. Hlawacek (c), H. Hoffmann (e), M. Ramsey (d), R. Resel (f), Q. Shen (c), C. Simbrunner (b), H. Sitter (b), C. Teichert (c), A. Track (d,f), G. Trimmel (a) and W. Kern (g)

Sub-micrometer channel length OTFTs with ultra-thin organic gate dielectrics by nanoimprint lithography

C. Auner, U. Haas, H. Gold, B. Stadlober, G. Jakopic, J. Krenn

Self assembled monolayers: A study of 11-mercaptoundecanoic acid on Au – surfaces

P. Frank (a), J. Stettner (a), T. Griesser (b), G. Trimmel (b), R. Schennach (a), R. Resel (a), A. Winkler (a)

The effect of self-assembled monolayers on the mobility and contact resistance in polymer FETS

F. Gholamrezaie (a), K. Asadi (a), E. C. P. Smits (a,b), P. Blom (a), B. de.Boer (a)

Hole injection barrier optimization at ITO/organic interfaces modified with strong molecular acceptors

R.-P. Blum (a), B. Bröker (a), S. Duhm (a), A. Vollmer (b), R. Rieger (c), H.J. Räder (c), K. Müllen (c), J.P. Rabe (a), N. Koch (a)

Adsorption of 1,4,5,8,9,12-hexaaza-triphenylene-2,3,6,7,10,11-hexacarbonitrile on Cu, Ag, and Au

O. T. Hofmann (a), G. Rangger (a), L. Romaner, (a), B. Bröker (b), R.-P. Blum (b), N. Koch (b), A. Vollmer (c), E. Zojer (a)

Theoretical and experimental studies of anthraceneselenol SAMs on Au(111)

A. M. Track (a,b), G. Heimel (c), D. Käfer (d), A. Bashir (d), G. Witte (d), E. Zojer(a)

Tuning of the interchain interaction and the photovoltaic performance in polymer-polymer blends

M. Schubert (a), C. Yin (a), S. Bange (a), B. Stiller (a), M. Castellani (a), D. Neher (a), C. Dosche (b), M. Kumke (b), H.-H. Hörhold (c)

Plasma polymerization mechanisms study: from the gas phase to the surface

X. Gillon, L. Houssiau, J-J. Pireaux

Investigation and modeling of the dielectric/semiconductor interface properties in organic field-effect transistors

E. Orgiu (a), M. Taki (a), A. Bonfiglio (a,b), B. Fraboni (c), E. Scavetta (d), S. Locci (a,b,e), G. Scarpa (e), C. Erlen (e), P. Lugli (e)

Morphology and OFET properties of poly(3,3'''-didodecyl-[2,2':5',2'':5'',2''']-quaterthiophene) (PQT-12) with different molecular weights

P. Pingel (a), A. Zen (b), B. Stiller (a), D. Neher (a), S. Allard (c), U. Scherf (c)

AFM and PEEM Study of the in-situ Growth of 6P on TiO₂ (110) and Cu (110) in UHV

A. J. Fleming, M. G. Ramsey

Rubrene thin film characteristics on Mica Substrate

Sh.M.Abd Al-Baqi (a), G.Hernandez-Sosa (a), H.Sitter (a), B. Th. Singh (b), Ph. Stadler (b), N. S. Sariciftci (b)

Modelling of charge carrier transport in semiconductors and semiconductor devices

K. Zojer, F. Schürrer

Charge transport in organic semiconductors: commonly used models and comparison to temperature dependent measurements in organic thin film transistors

A. W. Golubkov, P. Pacher, and E. Zojer

Nucleation-Governed Reversible Self-Assembly of an Organic Semiconductor at Surfaces: Long-Range Mass Transport Forming Giant Functional Fibers

R. C. Savage, G. De Luca, A. Liscio, P. Maccagnani, F. Nolde, V. Palermo, K. Müllen, P. Samorì

Influencing the growth of Pentacene with Langmuir Blodgett films

H. Etschmaier, P. Pacher, M. Weis, J. Cirak, A. Lex, H. –G. Flesch, R. Resel, A. Haase, G. Trimmel, and E. Zojer

Current density variations near the metal-semiconductor transition

P. Reuter and P. Hadley

Performance improvement of dye-sensitized solar cells based on multi-walled carbon nanotube composite materials

A. Chindaduang, T. Sawatsuk, W. Wongsukkab, S. Pratontep and G. Tumcharern

Universal Arrhenius temperature activated charge transport in diodes from disordered organic semiconductors

N. I. Craciun, J. Wildeman and P. W. M. Blom

Integrated organic sensor modules

E. Kraker, G. Jakopic, V. Schmidt, B. Lamprecht, C. Konrad, S. Köstler, A. Haase, and J. Krenn

Pentacene and para-sexiphenyl heterostructures on clean and oxygen reconstructed copper surfaces

M. Oehzelt (a), G. Koller (b), T. Haber (c), M. Koini (c), S. Berkebile (b), R. Resel (c), M.G. Ramsey (b)

All-organic magnetic molecules: synthesis, magnetic properties, and thin film growth

P. Campiglio (a), M. Campione (a), C. Canevali (a), F. Canepa (b), M.R. Cimberle (c), C. Fanciulli (d), L. Miozzo (a), M. Moret (a), A. Papagni (a), A. Sassella (a)

Material optimization for light emitting diodes

R.A.H.J. Kicken (a) S.Harkema(a), J Sweelssen(a), B. Langeveld(a), A. van Breemen(a), N. Meulendijks(a), H. Schoo(a), M. de Kok(b), R. Coehoorn(b,c), B. Meijer(c)

Materials for Organic Bulk Heterojunction Solar Cells and Sensor Applications

J. Sweelssen (a), M. Koetse (b)

Flexible Organic LEDs for Lighting and Signage

S. Harkema

Abstracts: Talks

Sunday: 8:30-9:20

Growth and electronic band structure of electronically active organic films

M.G. Ramsey

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Institute of Physics: Surface and Interface Physics, Karl-Franzens University Graz, Austria.

The ability to control the molecule/crystallite orientation and morphology of "semiconducting" molecules is on the one hand a prerequisite for optimizing organic device performance while, on the other, it is a necessary condition for the unambiguous determination of their physical properties. With examples from sexiphenyl (6P), sexithiophene (6T) and pentacene (5A) we will discuss the means of obtaining thick organic films with unique crystalline orientations and morphologies [1]. From the basis of these organic single crystal films the intra- and inter-molecular band structure of the all important upper π -bands will be presented [2]. Finally they are used as controlled substrates to investigate both organic- and inorganic- on-organic interface formation [3].

Acknowledgement: This work is supported by the Austrian Science Foundation FWF

References

- [1] M. Oehzelt, L. Grill, S. Berkebile, G. Koller, F. P. Netzer, M. G. Ramsey, Chem. Phys. Chem. 8(2007)1707
- [2] G. Koller, S. Berkebile, M. Oehzelt, P. Puschnig, C. Ambrosch-Draxl, F. P. Netzer, M. G. Ramsey, Science 317, 351 (2007)
- [3] Georg Koller, Stephen Berkebile, Joachim R. Krenn, Falko P. Netzer, Martin Oehzelt, Thomas Haber, Roland Resel, Michael G. Ramsey, Nano Letters 6(2006)1207

Sunday: 9:20-9:40

Metal work function tuning with new molecular acceptors

B. Bröker (a), R.-P. Blum (a), A. Vollmer (b), O. Hofmann (c), S. Duhm (a), H. Glowatzki (a), R. L. Johnson (d), R. Rieger (e), H. J. Räder (e), K. Müllen (e), J. P. Rabe (a), and N. Koch (a)

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(b) *Berliner Elektronenspeicherring-Gesellschaft für Synchrotronstrahlung mbH, D-12489 Berlin, Germany.*

(c) *Institut für Festkörperphysik, Technische Universität Graz, Petersgasse 16, A-8010 Graz, Austria.*

(d) *Institut für Experimentalphysik, Universität Hamburg, D-22761 Hamburg, Germany.*

(e) *Max Planck Institut für Polymerforschung, Ackermannweg 10, D-55128 Mainz, Germany.*

The morphology and electronic properties of interfaces between metal electrodes and electroactive organic materials are important for the performance of organic electronic devices. One way of optimizing the electronic structure at the anode/organic interface is pre-covering of the electrode with a (sub-)monolayer of molecular acceptors. Here we present an ultraviolet photoemission spectroscopy (UPS) study of new electron acceptor molecules deposited on Au(111), Cu(111) and Ag(111). The acceptors comprise different functional moieties: keto, nitro and cyano groups. This study intends to improve the understanding of how the interactions of specific electron withdrawing groups with metal surfaces are correlated with observed modifications of interfacial electron density distribution, work function change ($\Delta\phi$), and the energy level alignment. We find that $\Delta\phi$, which is the difference between the work function (ϕ) of the clean metal surface and ϕ after formation of a molecular monolayer, is a monotonic function of initial ϕ of the metal. Two different slopes were observed for acceptors with cyano groups and those with keto or nitro groups.

This work is financially supported by the European Community project "IControl" (EC-STREP-033197).

Sunday: 9:40-10:00

Contact formation on organic films: A tale of three inorganics

S. Berkebile, G. Koller, J. Ivanco, S. Fleming, F. P. Netzer, M. G. Ramsey

Institut für Physik, Karl-Franzens Universität, Graz

The issues of band alignment and wettability of various contact materials are addressed with in situ studies on crystalline sexiphenyl films with known molecular orientation. The contact materials considered range from “reactive” Ti to “unreactive” Al and “inert” LiF evaporated on the organic both in ultra-high vacuum (UHV) and in background pressures simulating the poor vacuum typical for device production. Ultraviolet photoemission spectroscopy (UPS) and work function measurements have been used for determining band alignment, x-ray photoemission spectroscopy (XPS) to access the “chemistry” at the interface and interdiffusion and near-edge x-ray absorption fine structure (NEXAFS) to estimate the degree to which the crystallinity of the film is disturbed. For Al, poor vacuum is shown to improve wettability and band alignment (for electron injection). In contrast, Ti in UHV makes a good contact in both of these respects, however oxygen background pressures stop the formation of the ultrathin carbide layer responsible for these desirable properties. The complex story of LiF, often used in “real” devices, will be discussed in the light of our results.

This work was supported by the FWF and the European Community - Research Infrastructure Action under the FP6 "Structuring the European Research Area" Programme (through the Integrated Infrastructure Initiative "Integrating Activity on Synchrotron and Free Electron Laser Science - Contract R II 3-CT-2004-506008").

Sunday: 10:30-11:20

Self-Assembled Monolayers

Gregor Witte

Physikalische Chemie I, Ruhr-Universität Bochum, Germany

Due to the huge number of organic compounds available today, organic materials and of course also the corresponding surfaces can be tailored to exhibit a variety of specific physico-chemical properties by choosing appropriate organic molecules. However, the fabrication of well defined organic surfaces with a high degree of structural order can be quite difficult. On the other hand since many surface properties such as wettability or the interaction with other materials (reaction, adhesion) are essentially determined by the chemical termination (i.e. the outermost molecular unit) monomolecular films are already sufficient to adjust such properties. A rather simple but versatile method of creating highly ordered monolayer films is based on the so-called “self assembly” process which is a spontaneous formation of ordered domains of covalently bound adsorbates upon immersion of solid substrates into appropriate solutions. After discovery of this self assembly mechanism for the case of disulfides on gold surfaces [1] in the early 80’s a large number of studies have been performed for organothiol-SAMs on noble metals which has become a prototype system which can be prepared easily from ethanolic solutions of low (typically milli-molar) concentrations. In addition corresponding anchoring units such as silanes or phosphonates have been used to also allow the formation of SAMs on SiO₂ or metal oxide surfaces, respectively.

In this talk, I provide a brief overview of the formation, structural properties and stability of such molecular films and discuss the various methods of preparation and their characterization [2-4]. Several examples will be presented which demonstrate the versatile application of SAMs ranging from lubricants to bio-recognition applications. While at the beginning primarily aliphatic alkanethiols have been used more recently aromatic SAMs have become the focus of interest due to their superior electronic properties which favors also potential applications as nano-resists in lithography or contact primers in organic electronic devices. Moreover, in combination with tunneling spectroscopy the use of highly ordered aromatic SAMs enables also microscopic charge transport measurements through monomolecular films.

[1] R.G. Nuzzo, D.L. Allara, J. Am. Chem. Soc. **105**, 4481 (1983).

[2] A. Ulman, Chem. Rev. **96**, 1533 (1996).

[3] F. Schreiber, Prog. Surf. Sci. **65**, 151 (2000).

[4] J.C. Love, L.A. Estroff, J.K. Kriebel, R.G. Nuzzo, G.M. Whitesides, Chem. Rev. **105**, 1103 (2005).

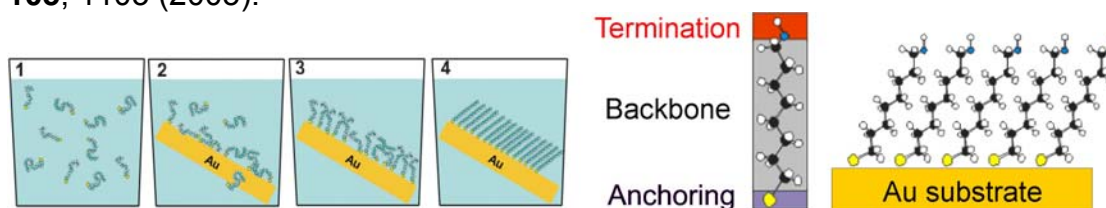


Abb 1. Schematic description of the formation of a self-assembled monolayer on an Au substrate upon immersion, together with the schematic architecture of a SAM for an organothiol.

Sunday: 11:20-11:40

Modifying electrodes in field-effect transistors by self-assembled monolayers

K. Asadi, F. Gholamrezaie, E. C. P. Smits, P. W. M. Blom, B. de Boer

Molecular Electronics, University of Groningen, FOM-G-15

Depending on the electronic dipole associated with the thiol molecules, which assembles themselves on gold surface and form a monolayer, the interfacial electronic properties are changed. We report a significant change in work function of gold by monolayers of two different alkanethiols. Analysis of the output and transfer characteristics of the organic field-effect transistors with modified source-drain electrodes with the monolayer, are presented. By using the right analysis, charge carrier mobility of the polymer, corrected for the contact resistance, is derived. We show that, despite some of the reports in literature, the mobility which is a property of the polymer is not influenced by the presence of the monolayer while the contact resistance is changed.

Sunday: 11:40-12:00

New Approach for Metallization of SAMs by making use of Electronegativity

D. Käfer, G. Witte

Daniel.Kaefer@rub.de

Physical Chemistry I, Ruhr-University Bochum, D-44780 Bochum, Germany.

Metal layer formation on top of a well defined non-conductive organic monolayer has been an important research subject in recent years as such systems will not only offer a promising approach to molecular electronics, but also may be used in organic electronics for the fabrication of microelectronic devices. SAMs of thiols on Au are good candidates to be used for this purpose because of their unique advantages such as formation of highly ordered structures and ability of tailoring surface properties by head group functionalization.

Despite numerous attempts of metallization by vapor deposition of e.g. Au, Ag, Cu,... on top of SAMs with different head group-functionalization, there have only been very few experiments like currentless deposition of Pd which seem to be successful in preventing the metal penetration through the SAM onto the Au, creating shorts.

In this study we have chosen a different driving force for keeping the metal atoms on top of the organic molecules: the electronegativity. By using a partial fluorinated Alkanethiol [F₃C(CF₂)₉(CH₂)₂SH] on Au as well-ordered substrate and evaporating Cs under UHV conditions upon this, the metal ions could be trapped by the fluorine atoms. This resulted in Cs atoms sticking around a fluorinated Alkanethiol or even in salt formation due to the high electronegativity difference of 3.2, and in C=C bond creation, as proven by photoelectron spectroscopy (NEXAFS, XPS, UPS) and infrared spectroscopy. The F1s-NEXAFS and IR measurements showed that a strong coupling between F and Cs must exist, whereas the lower hydrocarbon part is not affected. A penetration through the SAM is thus blocked by a clustering of Cs on top of the organic molecules as also seen in SEM images. Therefore, a true metallization can be reached by fixing the metal atoms to the thiol head groups electrostatically. The fixing mechanisms and the structure of the resulting film will be discussed in detail.

Sunday: 17:10-18:00

Quantum Mechanical Simulation of Self-Assembled Monolayers

G. HeimeI

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Self-assembled monolayers (SAMs) of organic molecules covalently bound to a variety of substrates are becoming an important tool to modify surface properties in general, and to optimize the electrode-organic interface in plastic electronics in particular. There, SAMs are employed to direct the growth and morphology of the active organic layers and, more importantly, to reduce the barriers for charge injection into the device and thus minimize its onset voltage. Moreover, SAMs can be used as devices in their own right, either with the whole monolayer carrying the device functionality or in the context of single-molecule electronics, where a single or a few molecules are the active element.

In the present tutorial, we will focus on SAMs on coinage metals. First, some basic concepts of metal-organic interfaces will be reviewed and their importance for organic electronics will be highlighted, allowing us to identify their most relevant properties. We will then provide a brief overview over the experimental techniques used to study these interfaces in order to understand, tune, and optimize their properties for applications in organic electronic devices. Against this background, a summary of available theoretical and computational approaches will be given with a focus on quantum-mechanical techniques. We will critically assess the reliability of these methods and discuss their role in understanding important interfacial and surface properties of SAMs. A number of experimentally accessible observables and their modeling will be discussed, including, e.g., photoelectron spectroscopy data, scanning tunneling microscopy images, and vibrational spectra. In particular, we seek to highlight what complementary information and what additional insight can be gained from quantum-mechanical calculations with the goal of establishing a comprehensive picture together with experiment.

Subsequently, the results from a detailed theoretical investigation of a prototypical class of molecules are presented in which the impact of every component of a SAM on the interface energetics is analyzed. These include the substrate metal, the docking group, non-conjugated spacers, the length of the conjugated core, and headgroup substitutions. Moreover, we highlight the effect of coverage on the interface energetics and give an outlook on the theoretical description of charge transport through single molecules and monolayers.

Sunday: 19:00-19:20

DFT calculations including van der Waals dispersion forces: PTCDA on Ag(111)

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A detailed understanding of the processes governing the adsorption of molecules on metallic surfaces is of major interest for the field of molecular electronics. Calculations of adsorbed molecules on the atomistic level can provide useful insights into such processes. For the theoretical description, density functional theory (DFT) in the framework of the generalized gradient correction (GGA) is widely in use. However, with this method, van der Waals dispersion interactions are not accounted for. Therefore, adsorption energies (distances) are typically underestimated (overestimated) by this method. The effect is of minor relevance for molecules which are covalently bound to the surface but play a major role for all weakly bound molecules for which, sometimes, DFT gives no binding at all in contrast to experiments. The prototype system of this sort is represented by the molecule 3,4,9,10-perylene-tetracarboxylic acid dianhydride (PTCDA) adsorbed on Ag(111) which has been extensively characterized by experiments and the binding distances to the surface have been determined by means of x-ray standing wave measurements.

In this contribution we present DFT calculations of PTCDA on Ag(111). We adopt a recently developed exchange-correlation functional which goes beyond GGA and has been explicitly designed to include van der Waals interactions. We will show that this method describes the binding of PTCDA in contrast to GGA and we discuss the relevant contributions to the total adsorption energy. This will be accompanied by an analysis of the occupation of the molecular orbitals of the adsorbed molecule.

Monday: 8:30-9:20

Advanced UPS studies of weakly interacting organic layers

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We will discuss some important issues related to the hole mobility of an organic thin film transistor using the results obtained with high resolution and “high-purity” UPS. The discussion is closely related to “construction” of a new pathway which links the UPS experiments more elegantly to physics of energetics and charge-transport properties in thin-film organic and molecular devices. Following topics will be discussed in the present talk:

- (1) HOMO-hole/molecular vibration coupling and related ultrafast phenomena, which must be considered in discussing the charge transport properties in organic thin films and through organic/conductor interfaces.
- (2) Intermolecular energy band dispersion and hole mobility.
- (3) Detection of intrinsic gap states of organic films by “high-purity” UPS and related phenomena including the energy level alignment.

Monday: 9:20-9:40

Zeno effect and step edge barrier in organic thin films

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Organic Semiconductors start to enter the market of consumer products as light emitting diodes, solar cells, and thin film transistors. For the growth of reliable high quality devices a profound understanding of the processes related to formation of organic thin films is necessary. Here, we present an AFM study on the growth of para-sexiphenyl on a ion-bombarded mica(001) surface. Para-sexiphenyl is a member of the group of small conjugated molecules with a high mobility [1] and the ability to emit blue light [2].

The morphology is characterized by the formation of mounds formed by upright standing molecules. Needle growth competes with the formation of the mounds. However, the characteristic layer distribution of the mounds can be fitted by a Poisson distribution. The cross sectional slope of the mounds is related to the Zeno effect known from inorganic epitaxy [3]. It has been analyzed for different film thicknesses. Furthermore, statistical roughness parameters such as rms roughness and mound separation have been evaluated. The growth exponent and dynamic exponent can be calculated and agree with the predictions made by the Zeno model. The mound separation and the size of the top terrace allow estimating the size of the Ehrlich-Schwöbel-Barrier responsible for the shape of the mounds.

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Monday: 9:40-10:00

The electronic structure of Pentacene/Fullerene layered and co-deposited thin films on poly(ethylenedioxythiophene): poly(styrenesulfonate) (PEDOT:PSS)

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The electronic structure of bilayer and vacuum co-deposited thin films of *the* prototypical p- and n-type organic semiconductors pentacene (PEN) and fullerene (C60) on the conducting polymer substrate poly(ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT:PSS) has been investigated by ultraviolet photoelectron spectroscopy (UPS).

For a film of C60 on PEN covered PEDOT:PSS an offset between the highest occupied molecular orbital (HOMO) levels of C60 and PEN of 1.7 eV was found. In this case, the PEN HOMO level was Fermi-level pinned with the onset of the photoemission at 0.35 eV binding energy (BE) and charge transfer between PEN and PEDOT:PSS lowered the sample work function by 0.7 eV, whereas the C60 HOMO level exhibited to be nearly vacuum level aligned. Interestingly, when reversing the deposition sequence to PEN on C60/PEDOT:PSS, the onset of the PEN HOMO level was 0.3 eV *above* the Fermi level, thus indicating a lack of thermodynamic equilibrium between the conducting polymer and the top PEN film. Co-deposited films (ratio 1:1) exhibit an offset between the highest occupied molecular orbital (HOMO) levels of PEN and C60 of 1.1 eV, which increased to 1.7 eV by pre-covering PEDOT:PSS with a thin pristine PEN layer, which equals the HOMO offset value found for pure C60 on PEN/PEDOT:PSS. In addition, the morphology and crystal structure of the respective systems have been investigated by means of atomic force microscopy (AFM) and x-ray diffraction (XRD), where we found pronounced phase separation of PEN and C60 in the co-evaporated films. XRD reveals crystalline growth of PEN in all investigated cases, whereas C60 was found to be crystalline only if grown on PEN covered PEDOT:PSS substrates. The investigated hetero-structures were successfully used for the fabrication of organic photovoltaic devices, and current-voltage (I-V) characteristics could be correlated with the physical properties derived from the complementary studies above.

Monday: 10:30-11:20

Organic Field Effect Transistors

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The main topic of this tutorial is the working mechanism of Organic Field Effect Transistors (OFETs). Following the interpretation key suggested by the school topic, we will focus on the role of interfaces in the device behavior.

We will see that this behavior is in fact mainly determined by several interfaces that play a very important role in the determination of transistor performances.

For instance, the interface between metal and organic semiconductors is important for determining the carrier injection in the channel: material properties and geometry of these interfaces are in fact responsible for the type and density of carriers in the channel.

Also the interface between the insulating layer and the semiconductor plays a major role, in particular, in charge trapping effects. Very recently this issue has been deeply discussed as a possible cause of the difficulty of obtaining n-type and ambipolar devices.

Mixed organic semiconductor layers may also be employed for realizing the active layer of OFETs. Therefore, they are again examples of material interfaces that may be employed for realizing high performance devices.

Finally, we will see an example of a field effect device used for making chemical sensing: in this case the interface between functional layers of the device and the external environment (in particular a liquid solution) is the key factor for obtaining such sensitivity.

Monday: 11:20-11:40

Controlling the characteristics of organic thin film transistors through interface modifications

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In this contribution we discuss two conceptionally different approaches to controlling the characteristics of organic thin film transistors (OTFTs) by modifying the properties of the interface between the active layer and either the dielectric or the metal electrodes.

In the first approach, a covalently bond reactive layer containing sulfonyl chloride and sulfonic acid groups is prepared on the surface of the SiO₂ gate dielectric prior to the deposition of the active layer (here, poly(3-hexylthiophene)). This results in a large positive turn-on voltage (V_T) of around 50 V. When exposing the device to a variety of amines (in particular to ammonia vapour), V_T shifts to negative voltages by approximately 65 V. This huge effect is caused by the interaction of the interfacial layer with the active material and is attributed to an efficient, localized chemical doping and dedoping mechanism, acting in close spatial proximity of the conducting channel. This process allows a switching of the device from depletion to accumulation mode and holds high promise for application in chemical sensing.

In the second set of experiments, we optimize the contact resistance in short-channel bottom-contact OTFTs (in this case based on pentacene) by a UV/ozone treatment of the Au electrodes. This procedure is highly effective in (i) decreasing the hole-injection barrier between Au and pentacene (as measured by photoelectron spectroscopy) and (ii) in improving the morphology of pentacene on top of the Au contacts. In this way, the contact resistance in our devices is reduced by an order of magnitude cm for gate voltages well above the threshold-reaching values as low as 80 Ohm and a channel-length independent carrier mobility in the range of 0.3cm²/Vs < μ < 0.4cm²/Vs is observed.

In both cases, an in-depth analysis of the interface properties turns out to be crucial for understanding the processes in the devices. Therefore, the interfaces were studies by numerous surface sensitive techniques including X-ray photoelectron spectroscopy, UV photoelectron spectroscopy, surface infrared absorption, and atomic force microscopy.

Monday: 11:20-11:40

Flexible Organic Field Effect Transistors with tunable threshold-voltage

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The emerging appealing possibility of exploiting organic heterojunctions for obtaining new electronics properties derived from the interface between different semiconductors is going to add a further degree of freedom for improving OFET performances. In this paper we report on the possibility to use organic bulk heterojunctions of two derivatives of a conjugated molecule for tuning and controlling charge carrier population and transport within the active layer. In particular, we report on the fabrication and operation of a series of OFETs, which exhibit (i) accumulation and depletion mode operation, (ii) wide tunability of threshold voltage, (iii) mechanical flexibility.

We fabricated OFETs on plastic substrates (Mylar®), acting at the same time as gate dielectric, by co-depositing two organic semiconductor materials, sexithiophene (6T) and α,ω -dihexylsexithiophene (DH6T), at various ratios. OFETs comprising pure 6T channels exhibited a slightly negative threshold voltage (V_T), thus working in p-type accumulation mode. When only DH6T formed the channel, large positive V_T was observed, giving evidence that an accumulation of p-type charge carriers was already present without applying any gate bias and that these OFETs work in the depletion regime. Photocurrent spectroscopy measurements confirmed that a larger concentration of charge carriers is present in DH6T OFETs.

For OFETs with mixed 6T:DH6T channels we found a linear dependence of V_T on the 6T: DH6T ratio. Moreover, the hole mobility was essentially constant for all mixing ratios ($\geq 5 \times 10^{-3} \text{ cm}^2/\text{Vs}$), and even higher than for pure 6T flexible OFETs ($3 \times 10^{-3} \text{ cm}^2/\text{Vs}$). X-ray diffraction and atomic force microscopy studies showed that 6T and DH6T co-deposited films (on Mylar® and Si-oxide) have very similar structural and morphological properties as the pure materials films, and that the two molecules form intercalation compounds. This is particularly interesting because it demonstrates the possibility to adjust the device working point and tune its operational mode without negatively affecting charge carriers transport across the channel.

Our work shows that extremely wide OFET function tunability can be achieved by combining molecules with appropriately adjusted properties in molecularly mixed films. A rational approach to precisely control OFET performance has thus been established, providing a considerable extension of the application-potential of organic electronics.

Monday: 17:10-18:00

Organic Light-Emitting Devices and Interface Tuning

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The emission of light from organic light-emitting diodes involves several elementary processes thus as charge injection, drift and recombination, the generation, diffusion and radiative decay of excitons and finally the outcoupling of light from the device structure. Efficient generation of light thus requires the optimisation of these processes, which is practically impossible for simple single-layer device architectures.

This tutorial talk gives an overview about strategies to understand and optimise the injection and recombination of charges by introducing defined organic-organic interfaces. Multilayer organic devices can be quite simply prepared by thermal evaporation. By optimising the device structure and the chemical composition of the used components, OLEDs with internal quantum efficiencies approaching unity have been demonstrated [1]. In contrast, multilayer processing from solution turns out to be quite difficult. Currently used approaches rely mostly on the self-assembly of molecules to tune the injecting of charges and the introduction of cross-linkable layers to tune the transport and recombination of charges [2]. More recently, a novel approach to insert ultrathin polymer layers with well-controllable electronic properties into solution-processed optoelectronic device structures has been proposed [3]. Upon proper choice of the HOMO and LUMO level of the interlayer material, efficient recombination of charges at the interface could be realized [4]. In my talk I will finally address the recombination of charges at and across such organic-organic heterojunctions and discuss approaches to tune this recombination process towards efficient generation of light.

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Monday: 19:00-19:20

Preparation and properties of parylene layers for OFETs

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Manipulating the semiconductor/dielectric interfacial properties via optimizing the gate dielectric can substantially enhance OFET performance. To this end, polymer dielectrics are ideal because of their diverse properties, favorable film-forming characteristics, and tunable surface chemistry for the control of device-critical interfacial trap state densities. Polymer dielectric chain dynamics affect organic semiconductor growth and OFET current-voltage (I-V) response.

Parylene's superior electrical insulation characteristics make it an excellent solution for the gate dielectric of OFETs.

We report on the fabrication and characterization of parylene gate dielectrics layers for organic field effect transistors (OFETs). Thin parylene layers will be deposited on the silicon dioxide surface under different growth rates. The structural and electrical properties of prepared layers will be characterized by ellipsometry to determine layer thickness homogeneity, atomic force microscopy to detect possible pin-holes and surface morphology and electrical investigations to determine the dielectric constants and electrical breakdown voltage. X-ray reflectivity will be employed to check the thickness homogeneity and surface roughness as well as X-ray diffraction to check the crystallinity and preferred orientation.

The pentacene OFETs with bottom contact structures will be prepared with parylene film as the gate insulator. Different parylene growth rate and surface treatment dependence on prepared OFET electrical properties will be reported.

Tuesday: 8:30-9:20

Functional macromolecules for organic electronics

Klaus Müllen

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A good case can be made when looking at Organic Electronic Materials by using modular repeat units such as the benzene or thiophene ring and connect them to different topologies. In that sense the size and the dimensionality of the molecules serve as design principles and guidelines of synthesis. Dimensionality leads to chain, disc and sphere-type structures and has, of course, a relevance for the dimensionality of charge transport processes in the solid. Typical chain-type conjugated polymers are poly-*para*-phenylene, polyphenylene vinylene and polyphenyleneethynylene which are synthesized by various carbon-carbon coupling techniques. More complex topologies such as conjugated macrocycles or disc-type graphene structures require more sophisticated methods whereby, however, the use of precursor polymers and templating are useful approaches. Charge transport and energy transfer processes in organic electronic materials occur in the bulk and at interfaces and often require a control of supramolecular order and solid-state morphology. That is why synthesis and processing (i.e. creating a well-defined macroscopic state of matter) must be looked at in a unified approach. Optimization of device performance does require the built-up of complex structural hierarchies which starts with the design of structurally perfect conjugated molecules.

Tuesday: 9:20-10:10

Organic chemistry as a tool for surface modification

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Skilled organic chemists with a solid background in Materials Science are nowadays capable to efficiently design and synthesize molecules and polymers with a wide range of interesting optical and electrical properties. The development of efficient structure-properties relationships in pi-conjugated materials in particular is boosting the emerging field of the molecular electronics, along with other interesting applications in research areas normally associated with standard inorganic semiconductors such as high speed telecommunication. The organization of these functional molecules into well defined supramolecular architecture, in particular in the form of thin films, represents however another level of challenge.

The self assembly of ordered monolayers or multilayers on properly modified inorganic surfaces represents one of the most efficient and fascinating strategies to prepare well characterized and well defined materials with a precise function, directly associated both with the chemical and physical properties of the deposited molecule and with the kind of the achieved order.

I will discuss various examples of chemical modification techniques aimed at the preparation of organic functionalized surfaces. In particular I will focus on the modification of oxide surfaces by chemical methods aimed at the definition of a precise reactive site. I will then discuss how the design of the functional molecular counterpart in the surface modification process has to be modified in order to account for the different environment the organics have in the solid state (interaction with the surface, interaction with neighbouring molecules). I will show in details how the precise definition of organic-inorganic interfaces is playing an important role in a number of technologically relevant devices such as electro-optic (EO) modulators, electrochromic devices, solar cells and OFETs.

Tuesday: 10:30-11:20

Fabrication techniques for organic electronics

E. List

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Tuesday: 11:20-11:40

Soft-landing mass spectrometry of rigid p systems for ordered and ultrapure layers for organic electronics

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In this investigation soft-landing mass spectrometry is proposed as a unique method for depositing ultrapure thin films of large aromatic molecules suitable for novel organic electronics. Via soft-landing the analyte molecules can be ionized, separated by mass to charge ratio through a mass analyzer and deposited with retention of their structures on a surface. As the analyte amount, which reaches the surface during soft-landing, is extremely low; soft-landing depositions have been so far used only for isolation of single polypeptides on a surface. This work demonstrates that ordered films of rigid rod molecules suitable for electronics can be obtained by employing a continuous ionization source, such as liquid secondary ion mass spectrometry (LSIMS), for increasing the amount of analyte collected on the deposition surface. Due to their high ionization/desorption efficiency and their suitability for novel organic electronics, dibenzo[b,b']thieno[2,3-f:5,4-f']-N-R-carbazole molecules are selected as a model system for this study. The molecules are ionized via liquid secondary ion mass spectrometry (LSIMS) and deposited on highly oriented pyrolytic graphite. The morphology of the ultra-pure single isotope [b,b']thieno[2,3-f:5,4-f']-N-R-carbazole films is studied via scanning tunneling microscopy (STM).

Furthermore, Dibenzo[b,b']thieno[2,3-f:5,4-f']-N-R-carbazole molecules are deposited on a carbon-covered copper support for performing transmission electron microscopy and electron diffraction analyses. The packing of the soft-landed molecules is compared to the packing of a reference drop-cast film. Their different molecular assembly is supposed to be related to the unique deposition conditions, which soft-landing allows. The strong electrical field, used to avoid fragmentation of the analyte ions reaching the surface, is supposed to affect the molecular order and the molecular packing of the analyte. To support this hypothesis, independent experiments are performed with the aim to study the electrical field influence on the molecular arrangement of non-polar extended aromatic p-systems, such as substituted hexabenzocoronene (HBC-PhC12), and more complex polymer structures, such as Poly(benzothiadiazole-co-cyclopentadithiophene).

Additionally, the soft-landing ability to form ordered films of molecules is tested by depositing thin organic layers on a bottom-gate, bottom-contact organic field effect transistor. The conditions for improved electronic performances are object of current investigations.

Tuesday: 11:40-12:00

Nanofibers from functionalised organic semiconductors

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The organic semiconductor *para*-hexaphenylene has proven to be a versatile building block for generating long, parallelly aligned organic nanofibers by a self-assembly process on a muscovite mica substrate via sublimation in high vacuum. They are extraordinary because of their properties such as intense, polarised fluorescence, which make them promising for integration in future submicron-sized optoelectronic devices. The challenge is now to have control over the nanofiber properties and morphology to widen the scope of possible applications. A powerful tool for that purpose is chemically functionalisation of the molecular building block, which will lead to an advanced modifying of the nanofibers and can even result in creating new properties. Functional groups have been implemented at the *para*-positions of *p*-quaterphenylenes using a non-trivial Suzuki cross-coupling strategy, and it is possible to grow well-shaped nanostructures from the new oligomers. The fluorescence peak emission frequency of the new nanofibers shifts within the blue and the overall shape alters depending on the functionalisation. Due to intrinsic non-zero hyperpolarisability of push-pull functionalised oligomers and non-centrosymmetry of the respective nanofibers, they act as frequency doublers.

Tuesday: 17:10-18:00

Structural characterisation of organic thin films

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We will discuss different approaches for the structural characterisation of organic thin films with emphasis on interface-sensitive X-ray scattering techniques, illustrated by a number of examples from the area of organic electronics and optoelectronics.

First, we will give a brief tutorial on X-ray reflectivity (specular and diffuse) for the study of film thickness and roughness as well as roughness correlations.

Second, we will explain the concept of grazing-incidence X-ray diffraction (GIXD) for the investigation of in-plane structures.

Third, we will introduce crystal truncation rods (CTRs).

Fourth, we will discuss X-ray standing waves (XSW) with photoelectron detection, which is a combination of a structural and a spectroscopic technique, with very high structural resolution in the monolayer regime, even element-resolved.

Examples will be shown from organic field-effect transistors (OFETs), encapsulation layers for devices, organic-organic heterostructures, and self-assembled monolayers (SAMs).

We will explain how the structural quality relates to device performance, how the interdiffusion of metal contacts into organics can be studied, and also how the film growth process can be monitored in situ and in real time.

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Tuesday: 19:00-19:20

Investigation of chemically and photochemically reactive siloxane thin layers for surface modification

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In this contribution we study two different types of siloxane thin layers able to undergo chemical and in the second case photochemical reactions. They can be used for the surface modification of silicon wafers. Layers comprising sulfonyl chloride and sulfonic acid moieties upon exposure to ammonia form the corresponding sulfon amide and ammonium sulfonate salt. We investigated this reaction in a siloxane thin layer by a variety of characterization techniques, such as contact angle (CA) measurements, zeta-potential measurements, X-ray photoelectron spectroscopy (XPS) and FTIR spectroscopy. The thickness of the layer is determined by X-ray reflectivity (XRR).

For the photoreactive thin layer we synthesized a trimethoxysilane molecule bearing the benzyl thiocyanate group that is known to undergo photoisomerization upon illumination with UV light to give the benzyl isocyanate compound. Contrary to the thiocyanate, the isothiocyanate can react in a post modification reaction with amino functionalized molecules to the corresponding thiourea compound. This provides the opportunity to prepare photopatterned surface layers with immobilized amine molecules only in the illuminated areas. The photoreaction as well as the post modification reaction is monitored by XPS and FTIR spectroscopy. The layer thickness is determined by XRR. Friction force microscopy (FFM) pictures of photopatterned and post modified surfaces show that a resolution down to a few micrometers can be achieved with lithographic techniques.

The herein presented chemically and photochemically reactive organic siloxane thin layers can be applied for tailoring surface properties of inorganic substrates and are, therefore, interesting candidates for interfacial layers in organic devices.

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Wednesday: 8:30-9:20

Scanning probe characterisation of organic layers

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Wednesday: 9:20-9:40

Application of ToF-SIMS and XPS in organic electronics

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Since about 20 years, Static Time of Flight Secondary Ion Mass Spectrometry is considered as a precious tool for organic material characterization because of its ability to provide molecular information with good spatial and mass resolution and extremely high sensitivity. Last year, attention rose for Dynamic ToF-SIMS and particular condition were obtained allowing keeping molecular information through layer depth and so to investigate diffusion, contamination, segregation or process reliability. In this work, we present results obtained in static mode on organic thin films and in dynamic mode with Caesium sputtering on OLED stacks. Several types of new and used pixels were investigated with different analysis conditions. XPS was also used as a complementary technique for quantitative atomic and binding information. Some XPS results on interest molecules are presented with an emphasis on a new acceptor type molecule.

This work is a part of the I-Control FP6 project funded by the European Commission (contract nr 033197).

Wednesday: 9:40-10:00

Depth profiling polymers and multi-layers with very low energy ions

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The need for molecular depth profiling technique to study organic layers has become a big challenge in the SIMS community in the last few years. Cluster ion beam (C₆₀⁺, Bin⁺...) depth profiling recorded some real success increasing hugely the secondary ions yields.

We investigated a different approach by using very low energy (down to 200eV) monoatomic (Cs⁺) or diatomic ions (O₂⁺). The very low energy allows to keep molecular information minimizing the polymer destruction. Also primary ions with great reactivity lead to an increase of the secondary ions fragments yields (especially anions for Cs⁺). Another approach was to take a look at the clusters formed by recombination above the surface of one or several cesium atoms (sputtered mostly positive) and molecular fragments. We not only found an echo of the negative spectrum in the clusters sub-spectrums, but also we were able to deduct some simple rules to characterize the clusters formation.

The use of low energy for sputtering was already known to perform ultra shallow depth profiles of inorganic material (impressive depth resolution for qualitative profiles). There is no doubt that this technique will also be applied for qualitative depth profiling of organic electronic devices providing information on interfaces (polymers multi-layers or metal/polymers interfaces).

Wednesday: 10:30-11:20

Optical characterisation of organics on surfaces

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It is well known that the electronic, transport and optical properties of thin organic films to be exploited in a variety of applications and devices may crucially depend on the structure and morphology of these films and their interfaces.

Therefore, it is important to understand the relationship between the thin film structure and interface morphology and the ensuing electronic and optical properties, preferably by monitoring them in an in-situ and online fashion during the growth or fabrication process.

We will demonstrate that optical techniques, in particular reflectance difference spectroscopy (RDS), provide a powerful means to investigate the structure and growth of thin organic films and, at the same time, to study the evolution of the electronic and optical properties in situ and with submonolayer sensitivity.

As examples, we discuss the growth of oligo-phenylenes and thiophenes (6P, 6T) on Cu and TiO₂ surfaces. We illustrate how the growth mode and structural parameters like the orientation of the molecules can be inferred from RD spectra probing substrate, thin film and interface related optical transitions. The shift, broadening and splitting of the characteristic HOMO-LUMO transitions can be monitored during growth and are related to changes in the electronic structure arising from the interaction of the molecules with the substrate and within the organic layer or from conformational changes of the individual molecules.

The RDS method also allows to resolve the fine structure of the main optical transitions, resulting from the strong electron phonon coupling in these films and to study its thickness and temperature dependence. Finally, structural phase transitions can be detected both as a function of coverage (i.e., during growth) and as a function of temperature.

Being a purely optical probe, RDS is not limited to UHV related fabrication processes but could, for instance, be applied to monitor the deposition from solution or to study organic thin film devices during operation.

Wednesday: 11:20-11:40

Low Temperature Study of The Exciton Diffusion in Conjugated Polymers

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The understanding of excitonic processes in organic semiconductors is extremely important both for the device operation and for the fundamental knowledge of the physics of this emerging class of materials. In particular, the exciton diffusion length is an essential parameter for the fabrication of efficient opto-electronic devices like photovoltaic cells [1] and light emitting diodes [2].

Soluble derivatives of polyphenylene-vinylene (PPV) were investigated by the means of time-resolved spectroscopy in the temperature range of 4-293K. Photoluminescence decay times of pristine PPV derivative thin films were compared with the one of heterostructured films. Such a heterostructure is formed by spin-casting the PPV derivative on top of an insoluble fullerene-based polymerized layer that act as an exciton quenching wall [3]. However, we demonstrated that the free interface of spin-coat MEH- and MDMO-PPV films also quenches excitons with efficiency comparable to the polymer-fullerene interface.

The relative exciton quenching efficiency as a function of the PPV thickness was calculated from the experimental data for different temperatures, and a 1D diffusion model was applied to extract both the exciton diffusion length and the diffusion coefficient in heterostructured samples. The temperature dependence of the exciton diffusion length (coefficient) for MDMO-PPV shows two temperature regimes with different trends. Upon cooling from the room temperature to 100 K the exciton diffusion length (coefficient) drops from 4,7 nm ($3,6 \times 10^{-4}$ cm²/s) to 2,9 nm ($1,5 \times 10^{-4}$ cm²/s). Further cooling down to 4 K leads to a weak temperature dependence and a slight growth up to 3,2 nm (2×10^{-4} cm²/s). The obtained results are qualitatively explained by the quasi-equilibrium exciton distribution in an inhomogeneously broadened density of excited states.

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Wednesday: 11:40-12:00

Possibilities of exohedral metallocomplexes of fullerenes for polymer solar cells

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Fullerenes are indispensable components of high-efficient plastic solar cells. Nevertheless, optimization of the fullerene properties has been paid much less attention than that of the polymer component. Recent work in the field suggests that, in addition to enhancement of solar light absorption by the active layer, one of the main possibilities of improving the plastic solar cell performance can be associated with increase of the LUMO energy of the fullerene acceptor that should result in increasing the open circuit voltage. In this work, we study exohedral metallocomplexes of C₆₀ with Os and Ir as potential acceptors for plastic solar cells. First, these metallofullerenes have essentially stronger optical absorption than pristine C₆₀ specifically in the range where conjugated polymers are usually transparent, i.e. below 2 eV. Therefore, more efficient harvesting of solar energy in the polymer cell is possible. Second, the LUMO energy of the metallofullerenes is less than C₆₀ by about 0.4 V that gives a possibility to increase the open circuit voltage. Third, the metal ligands can provide high solubility. In blend with a model conjugated polymer, MEH-PPV, the metallofullerenes effectively quench MEH-PPV photoluminescence and result in appearance of long-lived charged states (polarons) at MEH-PPV. Possibilities of metallofullerenes for polymer solar cells are discussed.

Wednesday: 17:10-18:00

Modelling Organic/Metal Interfaces

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This talk will describe our approach to the energy level alignment at interfaces of organic semiconductors in terms of Charge Neutrality Levels (CNLs). The CNLs act as the electronegativity or effective Fermi level of the organic material at the interface, and tend to align with the metal work function (metal/organic) or with the other CNL (organic/organic junction).

The position of the CNL can be calculated from the electronic structure of the molecule at the interface; since the gap is underestimated in DFT, we consider many-body corrections to the molecular energy when an electron is added to or extracted from a particular molecular orbital of the system. These result in shifts of the molecular levels and have the effect of shuffling the occupied and empty parts of the spectrum and increasing the molecular gap with respect to DFT. The CNL position for the organic material is then obtained either by integrating the DOS (induced through the interaction at the interface) or from the 'branch point' of the molecular Greens function. In this way, we are able to extract what we believe is an important parameter for the energy level alignment (the CNL) from a simple, fast calculation. The screening parameters at the interface, which also affect molecular level offsets, can be estimated from the static dielectric functions of the organic materials.

Results for junctions containing these materials will be presented, comparing induced dipoles and interface properties with experiment. Our work suggests that, at interfaces where the exact details of the interaction are not important, the CNLs are important quantities and that the CNL picture represents a general and intuitive model for understanding organic semiconductor interfaces.

Wednesday: 19:00-19:20

Bonding of organic acceptors on coinage metals – combining theory and experiment.

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The physical and chemical properties of organic/metal interfaces are of high interest for the application of molecular (sub) monolayers to modify surface properties. Interesting applications might be found in the field of molecular electronics, chemical sensing as well as the tuning of the injection barrier in organic electronic devices.

In this contribution we present a joint theoretical and experimental study of the strong acceptor F4TCNQ adsorbed on Cu (111) and Au (111). There, the electronic and structural properties were investigated by ultraviolet photoelectron spectroscopy (UPS) and X-ray standing wave (XSW) measurements. F4TCNQ adsorbs in a heavily distorted conformation accompanied by pronounced changes in the UPS spectrum and an increase of the surface work function. To gain deeper insight into the nature of the bonding between metal and molecule, the interface was modelled by means of density-functional theory based band-structure calculations. This allows a precise analysis of the interfacial charge re-arrangement upon monolayer formation.

Analyzing the crystal-orbital overlap population (COOP) and via projecting the orbitals of the isolated molecule onto the states of the metal/monolayer system we find forward-donation from the lone pairs of the molecule into the metallic states and back-donation from the metal into the LUMO of the molecule. The formation of a dipole layer upon adsorption in combination with the intrinsic dipole moment of the molecules determines the total work function. The density of states in the molecular region, the work-function modification, and the geometric distortion of the molecule upon adsorption can be directly compared to the experimental data. Calculated observables like infrared (IR) spectra as well as scanning tunnelling microscopy (STM) images allow establishing a more general picture of the complex interface energetics. The model systems F4TCNQ on Cu and Au are compared with F4TCNQ on Ag and calculations of Pyrenetetrone on the different coinage metals.

This work is financially supported by the European Community project "IControl" (EC-STREP-033197).

Thursday: 8:30-9:20

The Role of Interfaces for Device Degradation

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The degradation of thin film electronic devices such as diodes, transistors, and capacitors is very often a consequence of irreproducible damages of the transport relevant interfaces, which is true not only in organic thin film electronics but also in conventional silicon-based microelectronics. The device degradation can be induced either (i) by external stress from ambient influences including storage under extreme temperature conditions, temperature fluctuations, increased humidity, UV-light irradiation, ozone or oxygen atmosphere, introduction and migration of impurities or (ii) by internal stress due to device operation under conditions that are close to the maximum allowed values of vertical and lateral electric fields, forward and reverse current densities and power consumption.

External stress factors mainly affect the bulk of the material layers although disturbances of the interfaces are often involved, too. In many cases these shelf lifetime limiting external effects can be reduced or some of them even suppressed by appropriate passivation and encapsulation of organic electronic devices. The situation is different for degradations induced by stress at maximum operation conditions (operational stress), where mainly the interfaces are affected. As the charge carrier dynamics and therefore also the charge carrier transport in the devices is significantly determined and controlled by the interface between semiconductors and dielectrics as well as semiconductors and electrodes, it is of major importance to understand the detailed mechanisms of such degradation processes. In many cases interface trap states are involved as well as grain boundaries, interface dipoles or Schottky barriers.

In this talk operational stress damage effects that are known from standard silicon field-effect transistors will be revised and compared to degradations observed in organic thin film transistors. Usual stress conditions will be explained, characterization techniques that are sensible to interface damage will be introduced and the results discussed. There exists a broad range of models for interface degradation in organic thin film transistors with the more popular ones being discussed here.

Thursday: 9:20-9:40

Structure and Morphology of Conducting Polymerfilms for Photovoltaic Application

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Conducting polymers have shown to be interesting candidates for photovoltaics due to their high absorption coefficient, easy processability, mechanical flexibility and low costs. Furthermore the possibility to tune the properties of the polymers makes a broad application feasible. Nevertheless there are stringent constraints in device fabrication due to the short exciton diffusion length, i.e. the charge carrier separation has to occur in this length scale. Therefore the structure of the polymerfilm is crucial. It was shown that a blended structure compared to a layered structure increases the efficiency [1].

In the presented work we focus on such blend films. Two conducting polymers of different classes, of poly(phenylene vinylene) (PPV) and polythiophene (PT) derivatives, are blended with different ratios. Films are prepared by using spin coating. With optical spectroscopy (UV/Vis and FT-IR) the absorbed part of the optical spectrum and the stability under ambient conditions is detected. The structure and morphology of the films are investigated with scattering methods (GI(U)SAXS) [2] and the critical blending ratio for the bicontinuous structure is determined. In addition the secondary influence of the substrate and the contact on the film structure is investigated.

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Thursday: 9:40-10:00

Organic photodiodes on printed ITO coatings for flexible organic photodiodes

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In this paper we describe the fabrication of organic photodiodes on solution cast ITO bottom electrodes. ITO (tin doped indium oxide) coatings of a sheet resistance of 2 to 3 k Ω □ were produced by gravure printing process on PET and PEN substrates. The sheet resistance could be decreased by heat treatment at 120°C under reducing gas atmosphere (Ar₂/H₂) to 1 k Ω □. The transmission of the ITO coated PET films is more than 80 % in the visible range. The printing paste consisted of ITO nanoparticles which were dispersed in a solvent by using a surfactant. The dispersion was mixed with a binder and a photo initiator before printing. The printed films were hardened under UV-irradiation at low temperatures (< 130°C).

The ITO films were directly used as the first layer in an organic photodiode (OPD) stack.

The setup of the OPDs originates from the well known Tang photodiode, consisting of a stacked layer of copper phthalocyanine (p-type material) and perylene tetracarboxylic bisbenzimidazole (n-type material). An additional layer of Alq₃ (n-type material, protection layer against humidity and oxygen, blocking layer in matters of diffusion of cathode atoms into active layer during deposition) is inserted to improve the charge carrier injection from the cathode (Al). The photodiodes are characterised via I/V characteristics as well as external quantum efficiency measurements. The performance of the photodiodes with printed ITO on plastic substrates is comparable to the performance of photodiodes with semi-transparent gold as anode on glass substrates. These results demonstrate the suitability of the printed ITO layers as anode for organic photodiodes. The performance could even be improved by the addition of a smoothing layer of PEDOT (Baytron) on the ITO substrates.

The ITO layers have been investigated by AFM with respect to roughness investigations and with ellipsometry for the determination of the optical constants. The electric conductivity of the ITO layers has been altered by additional UV treatments and by reducing atmosphere. The conductivity mechanisms in the ITO and the ITO/PEDOT double layers have been investigated by XPS and transmission measurements.

Thursday: 10:30-11:20

Using Transmission Electron Microscopy to analyze the structure and morphology of organic functional materials

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Transmission Electron Microscopy (TEM) is a unique and powerful tool for the morphological and structural analysis of functional organic materials. This is due to the possibility to observe by TEM a given object of submicrometric size in both real space and reciprocal space. TEM can therefore provide valuable informations on both morphology (domain size, anisotropy, connectivity, etc...) and structure (orientation, contact plane, presence of defects, etc...). I will first make a brief introduction to the technique itself, explaining the different observation modes (bright field, electron diffraction, dark field, tomography) as well as the possible sample preparation methods. I will then take a given number of examples on key organic molecular and polymeric materials (pentacene, regioregular poly(3-alkylthiophene), etc...) illustrating the importance of TEM in the structural analysis of organic functional materials.

Thursday: 11:20-11:40

Structural properties of sexiphenyl / pentacene / sexithiophene triple layer organic heterostructure on a Cu(110)-(2x1)O surface

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A triple heterostructure of 30nm sexiphenyl, 30nm pentacene and 20 nm sexithiophene was grown on a Cu(110)-(2x1)O surface under UHV conditions and was investigated during the growth procedure *in-situ* by NEXAFS. Additionally, the triple heterostructure was investigated by *ex-situ* XRD. The NEXAFS investigations reveal – within the relatively large uncertainty of the method - that the sexiphenyl molecules within the first layer on the Cu(110)-(2x1)O surface are aligned with their long molecular axes along the oxygen rows of the substrate. The pentacene molecules in the next layer as well as the sexithiophene layer in the third layer have the same alignment of the long molecular axes and orientation of the aromatic planes as the sexiphenyl molecules in the first layer: a uniaxially oriented triple heterostructure was grown.

X-ray diffraction using pole figure technique reveals the alignment and orientation of the molecules in the crystalline bulk state as they are present in the 30 and 20nm layer of the triple heterostructure. The alignment and orientation of the molecules of the NEXAFS investigations could be confirmed. The crystallographic planes parallel to the substrate are (20-3) for sexiphenyl, (022) for pentacene and (010) for sexithiophene with epitaxial relations such that all long molecular axes are parallel to the oxygen rows. A reciprocal space map across the specular diffraction peaks reveals no difference in the mosaicity of the crystals of the three organic layers. However, the mosaicity of the crystals along and perpendicular to the oxygen rows (even within one organic layer) differ and will be discussed. The investigations suggest the driving mechanism in the formation of epitaxially ordered organic layers above an ordered organic surface. Individual molecules and/or molecular clusters of the top layer match with the van der Waals surfaces of the layer below, a mechanism which is already predicted for the heteroepitaxial growth of polymers.

Thursday: 11:40-12:00

Epitaxial Order of Pentacene on Cu(110)-(2x1)O induced by Surface Corrugation

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In this study, the structure of a 30 nm thick pentacene film grown by molecular beam deposition on an oxygen passivated Cu(110) single crystal has been investigated ex-situ by x-ray diffraction methods. It is shown that pentacene crystallizes in two known bulk polymorphs with four unique crystal orientations. The Holmes phase with the (022) plane parallel to the substrate surface is observed to be dominant. In all four cases it is found, that the surface corrugation of the atomically ordered two fold symmetric Cu(110)-(2x1)O substrate aligns the pentacene crystallites so that a principle pentacene direction is parallel to the substrate corrugation. Unlike the epitaxial ordering through lattice matching achieved in previous studies, the crystallite ordering of pentacene on Cu(110)-(2x1)O is found to be driven by a novel criterion: The alignment of major crystallographic directions of pentacene with the substrate surface corrugation.

Thursday: 17:10-18:00

Challenges for the industrial realization of organic electronics

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In the past decades applications of organic electronics have progressed from laboratory curiosities to potentially marketable products with sufficient benefits to penetrate existing markets and create new ones. Some applications are currently being marketed, such as OLEDs, electrochromic and -phoretic displays and thin film batteries, but have generally not yet reached the point that the market is willing to replace its existing products. Organic Electronics can be called a key technology of the 21st century that enables new applications and opens up new markets. This is recognized by many companies, research institutes, universities and consortia that aim to improve those aspects of organic electronics that need to be overcome to mature these technologies.

The challenges that exist may be different between applications. For organic field-effect transistors, for instance, the challenge is to develop p- and n-semiconductor materials with high mobilities and a high shelf-life and operational lifetime. Furthermore, it is highly beneficial if these materials are solution processable and can be deposited in a cost-efficient manner on large scale. With mobilities several orders of magnitude lower than amorphous silicon, achieving these goals can be considered a necessity.

Inorganic photovoltaic cells reach power-efficiencies up to four times as high as the best organic solar cells to date. For organic photovoltaic cells, the challenges thus also concern material aspects as well as processing issues. From a more fundamental point of view, exciton generation, diffusion, dissociation and charge carrier transport to the electrodes are currently intensively investigated. From a processing point of view, the challenge is to transfer the processes to flexible substrates and while increasing the active area still maintain high efficiencies and operational lifetimes.

Many of the same challenges exist for another organic electronics application, namely the organic light-emitting diode. It is estimated that approximately 20% of global energy consumption is for lighting, signage and signaling. The development of inorganic and organic light-emitting diode (LED and OLED) applications is thought to coincide with large savings in costs, and energy consumption. The OLED and its inorganic counterpart have the potential to replace the incandescent as well as the more efficient (compact) fluorescent lamps once their efficiencies, costs of ownership, lifetimes, color, color temperatures and color rendering, have reached the necessary levels. However, the status today is that many issues need to be resolved before it is possible to coat our buildings with large tiles of OLED lighting or to replace the headlights of our cars with high-power LEDs. To achieve a cost-effective and sufficiently large scale production scheme for OLED lighting, signage, display and signaling applications, the choices are to increase the size of the substrate to several square meters and / or to transfer the processes to a roll-to-roll production line. This will require unprecedented accuracy of material deposition and patterning and innovative device and system concepts.

In our contribution we will present the general and more application specific challenges that exist for organic electronics when transferring the manufacturing process from a laboratory scale to an industrial scale.

Abstracts: POSTERS

Nanostructured and highly oriented polycarbonate layers

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Polymer surfaces showing a periodic relief structure or a high degree of polymer chain orientation are widely used in the fabrication of technological objects e.g. compact disks, liquid crystal displays and anti-reflective coatings. Rubbing is a widespread method to prepare alignment layers, but the surface of rubbed films is usually very high and incompatible with certain applications e.g. the design of organic field effect transistors. Herein, we present a simple and versatile method to prepare alignment layers which combine a controlled surface roughness, a periodic nanostructured polymer surfaces and a high degree of polymer chain orientation. The nanostructuring of the polymer layers implies the alternation of crystalline polymer lamellae in edge-on orientation and amorphous interlamellar zones (20 nm periodicity). The process described herein involves three steps: i) the preparation of a polymer film in its glassy state, ii) the near-surface orientation of the polymer chains by rubbing and iii) a solvent induced plastization and crystallization. As an example, we demonstrate that polymer surfaces of bisphenol A polycarbonate (PC) produced by this method exhibit a very high orienting ability for a large class of materials e.g. zinc phthalocyanine and bis-azo dyes. ZnPc nanocrystallites are oriented parallel to the crystalline lamellae of the PC substrate. The level of orientation is closely related to the average surface roughness of the nanocorrugated PC layers which is controlled by the crystallization time of the PC films.

Brinkmann and J.-C. Wittmann, Fr. Pat. n°2 891 187, 2005

Polymer Thin Film Characterization: A Combined Approach by X-ray Reflectivity And Spectroscopic Ellipsometry

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Thin films of different polymers are used for a combined characterization approach performed by x-ray reflectivity (XRR), spectroscopic ellipsometry (SE) and atomic force microscopy (AFM). The quantities of interest are film thickness, surface and interface roughness, electron density of the layers and the optical constants of the materials in the thin film regime. XRR yields the film thickness with high accuracy; additionally for electron density and surface as well as interface roughness are derived from simulations (Software: WinGixa) which do not provide unique results. SE evaluation (Software: WVASE) provides the layer thickness, roughness, refractive index and absorption coefficient in the spectral range from UV to IR. Both techniques, XRR and SE can only be evaluated if some knowledge about the system is provided in advance as for example the sequence of the layer structure. A combined approach uses the layer thickness determined by XRR as an input parameter for the simulation of the SE measurements. As cross-check for the surface roughness atomic force microscopy is used.

Thermally oxidized silicon oxide is used as substrate for thin films of polystyrene and polyimide which are prepared by spin coating from solution and parylene films which are deposited from vapour phase. The polystyrene films are in the range from a few nanometres up to 200nm, and surface roughness up to 4nm. Especially the refractive index of polystyrene varies strongly in this regime [1]. On the polyimide films in-situ temperature experiments using XRR are performed to investigate the change in electron density and layer thickness during the imidization process [2]. The electron density increases and the layer thickness decreases from about 60nm to 30nm during the temperature treatment. The parylene films are investigated in a range from 5nm to 50nm for the layer thickness having a roughness of approximately 1 nm depending on the parameters during the preparation process.

It is shown that the combined approach provides a more accurate characterization of thin films giving results for the layer thickness, surface and interface roughness by XRR, refractive index and absorption coefficient by SE and a reference of surface morphology by AFM.

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Self Assembly of Multicomponent Nanostructures Driven by Hydrogen-Bond

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Functional surfaces can be developed by self-assembly of properly designed molecular building blocks forming two dimensional nanostructures with pre-programmed order at the supramolecular level. Hydrogen bonding can be successfully employed for this purpose taking advantage of its high directionality and selectivity. Here we report on the formation of several types of multicomponent monolayers, the assembly of which was directed by the use of specific hydrogen bonding units integrated in the chemical structure of the molecules. We characterised these systems at the sub-molecular level by means of scanning tunnelling microscopy (STM) at the liquid-solid interface. The STM results show a strong correlation between the orientation of the different hydrogen bonding sites in the molecules and the obtained molecular arrangements. This approach enables us to grow well defined multicomponents 2D nanostructures in a versatile way by varying the size and geometry of the molecular building blocks. Particularly we demonstrated the possibility to form nanoporous self-assembled structures each pore constituting a receptor site for the further deposition of functional molecules.

Depolarization Effects in Self-Assembled Monolayers:

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Many experimental and theoretical studies have demonstrated that the work function of metallic surfaces can be modulated by depositing onto them a dense two-dimensional array of polar molecules (i.e., a self-assembled monolayer, SAM); in turn, this modulates the barrier for hole and electron injection in opto-electronic devices such organic light emitting diodes and field-effect transistors [1-2]. The influence of the orientation of the molecules and size of the dipole on the vacuum level shift has been widely studied whereas a little attention has been paid to depolarization effects.

Our goal is to characterize the extent of depolarization effects (i.e., the evolution of the molecular dipole moment going from the gas-phase to the SAM) on the basis of quantum-chemical calculation by varying several molecular parameters. We focus exclusively here on the molecular component of the interface dipole and do not consider the contribution arising from the metal/organic interface [3]. Three different molecules have been considered; they include a thiol and a nitro group as terminal substituents and a spacer containing six carbon atoms, i.e., a phenylene ring, three double C-C bonds, and three dimethylene units.

For each molecule, we have characterized the evolution of the molecular dipole moment by building one- and two-dimensional clusters. The influence of the cluster density and geometry (by varying the tilt angle and rotational angle of the molecules) has been studied. The impact of the molecular size was also considered by increasing the length of the spacer. All together, the results point to significant depolarization effects (up to 30% for the systems considered) [4]; the latter have thus to be fully taken into account in simple models developed to rationalize at a quantitative level the amplitude of vacuum level shifts.

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Localized charge transfer in a molecularly doped conducting polymer

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Conjugated polymers can be rendered highly conductive upon doping, and are thus important for the further development of all-organic opto-electronic devices. However, very little is known about the nature of donor/acceptor charge transfer in molecularly doped conjugated polymers. We have investigated the electronic structure in donor/acceptor polymer mixtures by N 1s NEXAFS spectroscopy in a 1 atm Helium environment, allowing us to investigate humid, spin-coated samples. We present evidence for a highly localized interaction between the prototypical organic donor poly(3-hexylthiophene) (P3HT) and the molecular acceptor tetrafluoro-tetracyanoquinodimethane (F4TCNQ) in thin films. Charge transfer leads to significant molecular distortions and a distinct self-localization of the new hybrid energy levels on a short single polymer chain segment. Design strategies towards high conductivity all-organic conducting polymers are derived from these results.

Novel Copolymers as semiconducting material for OFETs and OPVs

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During the last few years, the development of organic semiconductors as small molecules and polymers for application in organic field effect transistors (OFETs) and organic photovoltaic cells (OPVs) has gained increasing attention. There are many new materials with very high charge carrier mobility. Recently, naphthalene-bisimide, one of the earliest applied small molecule organic semiconductors, has been attracted considerable interest as an n-type material. Moreover, this small molecule is relatively insoluble in organic solvent and inflexible compared to the polymer. Recently reported novel naphthalene-bisimide based copolymer. This copolymer has been synthesised in an aryl-aryl-coupling according to Suzuki using Pd(PPh₃)₄ as catalyst. This copolymer can be solubilised in common solvent such as chloroform. The absorption spectrum shows two wavelength absorption maxima at ca. 386 nm and 606 nm. Further investigations should evaluate the potential of this novel copolymer as active component in electronic devices, especially as semiconducting layers in OFETs, and OPVs.

Synthetic strategies towards large planar acceptors for organic electronics

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For optimal interaction of organic molecules on metal surfaces large planar structures with LUMOs of low energy are needed. Four different approaches are presented here to achieve this goal: K-region oxidation of polycyclic aromatic hydrocarbons leads to very electron poor diketons, nitration and cyanation reduce the electron density of the molecule backbone effectively. Quinoid structures are focused on due to their strong tendency to aromatize by accepting electrons. Combinations of these methods lead to highly effective acceptor molecules which strongly interact with metals.

Nucleation-Governed Reversible Self-Assembly of an Organic Semiconductor at Surfaces: Long-Range Mass Transport Forming Giant Functional Fibers

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The controlled growth of highly stable, micrometer long supramolecular wires from a perylenebis(dicarboximide) with branched alkyl chains (PDI2) was achieved making use of solvent vapour annealing (SVA). During this process drop- or spin-cast thin films were kept above room temperature whilst exposed to a solvent-saturated atmosphere. Control of the parameters, such as choice of substrate, solvent concentration and temperature during SVA, affects various aspects of the resultant structures, e.g. aspect ratio and isotropic character. The growth was found to be a nucleation-governed process which complies with an Avrami-type of mechanism. The self-assembly into the wires was shown to feature a reversible character in which the formation of fibers could be favoured or hindered cyclically by using different solvents. Such versatility can potentially allow self-healing.

Atomic Force Microscope imaging after SVA showed that all the material deposited on the surface coalesced into the wires during SVA, leaving a bare surface of many hundred microns between fibres. This indicates a very high surface mobility of the PDI2 molecules during the annealing process.

The wires were grown on a wide range of surfaces, e.g. SiO_x, mica, gold and graphite, and were further seen to not be affected by surface roughness, thus allowing wires to be grown on electrodes. Preliminary I-V measurements on electrodes before and after SVA showed improved conductivity following the formation of wires.

These results make these supramolecular structures attractive for applications in (opto)electronics. The simplicity and versatility of the production method, coupled with the stability of the resultant wires, could be developed into simple, controllable and large-scale production methods for microelectronics.

AFM, Ellipsometry, XPS and TEM on ultra-thin oxide/polymer nanocomposit layers in organic thin film transistors

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We report on the fabrication and characterization of ultra-thin nanocomposit layers used as gate dielectric in low-voltage and high performance flexible organic thin film transistors (oTFTs). Reactive sputtered zirconia layers were deposited with low thermal exposure of the substrate. The resulting porous oxide-films with high leakage currents were spin-coated with an additional polymer layer like poly- α -methylstyrene (P α MS) or poly-vinyl-cinnamate (PVCi). After this treatment a strong improvement of the oTFT performance could be observed, leakage currents could be eliminated almost completely. In ellipsometric studies a higher refractive index of the ZrO₂/P α MS-layers compared to the “as-sputtered” zirconia films could be detected without a significant enhancement of the film thickness. Atomic force microscopic (AFM) measurements of the surface topography clearly showed a surface smoothing after the polymer coating. Further studies with x-ray photoelectron spectroscopy (XPS) and transmission electron microscopy (TEM) also indicated, that the polymer did not form an extra layer. The polymer chains rather (self-) assemble in the nano-scaled interspaces of the porous oxide film giving an oxide-polymer “nanocomposit” with a high oxide filling grade resulting in high dielectric constants larger than 15. The dielectric strength of more than 1 MV/cm is in good accordance with the polymer filled interspaces.

Packing of planar organic molecules: interplay of van der Waals and electrostatic interaction

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The molecular packing of pentacene and its two oxo-derivatives (6,13-pentacenedione and 5,7,12,14-pentacenetetrone) in their crystalline phase have been analyzed and compared with quantum chemical calculations of the electronic structure of the molecular entities. While pentacene reveals a face-on-edge herringbone packing, both oxygen containing species adopt an almost coplanar stacking. Quantum chemical calculations reveal a discernible charge localization at the oxygen atoms which in turn causes an electrostatic O-p-interaction and hence favors a planar stacking. On the other hand, the polarizability of the conjugated systems of both oxo-species is reduced which leads to a lower van-der Waals interaction and explains the small difference in the thermal stability of all studied oligoacenes. The present study emphasizes the importance of the balance of electrostatic and van-der Waals interactions.

Energy transfer in organic system of conjugated polymer and its ground-state charge transfer complex

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Blends of conjugated polymers and organic acceptors are actively studied systems as they can provide efficient dissociation of excitons into free charges. This process is of key importance for efficient organic photovoltaics. The energy migration through the polymer pi-conjugated segments into the lowest energy sites precedes charge separation in conjugated polymers. Energy migration is very effective due to the intrinsic intra-chain excitons delocalization and multichromophoric nanostructure of the polymer. Exciton dissociation and charge separation occur at the moment of an occasional meeting of a diffusing exciton and an acceptor molecule. One can expect that charge separation could be more effective in donor acceptor blends in which ground state charge transfer complex (CTC) between the donor and the acceptor is formed. Recently we have found that well known conjugated polymer MEH-PPV can form a ground state charge transfer complex with some organic acceptor molecules such as dinitroantraquinone (DNAQ) or trinitrofluorenone (TNF). In these blends a directional exciton transfer to the CTC is possible due to its low energy level. This directivity can provide higher efficiency of the following charge separation.

In this work energy transfer in the CTC forming blend of conjugated polymer and organic acceptor is studied by photoluminescence (PL) because PL can directly monitor the population of conjugated polymer singlet excitons. In the donor-acceptor blends with CTC the efficient PL quenching of MEH-PPV was observed at the low acceptor concentration (below 0.1%). We suppose that the efficient PL quenching results from the presence of the CTC. We build a model of Forster resonant energy transfer as a major quenching mechanism and we apply the model to our experimental data in solid films and solutions.

PL quenching in the blend of donor and low molecular acceptor in solution is known to be described by two general mechanisms: (1) static quenching through the formation of the CTC between the donor and acceptor, and (2) dynamic quenching through diffusive collisions between them. However, these mechanisms do not explain the observed efficiency of PL quenching in MEH-PPV/TNF. On the other hand PL quenching in polymer films doped with low-molecular acceptor can be described by Forster resonant energy transfer (FRET) model.

Unlike individual acceptor absorbing in the UV range, the CTC fulfils the general condition for efficient FRET due to overlapping of the characteristic CTC absorption band with the polymer PL spectrum. It is supposed that FRET can provide an energy funnel to CTC for excitons residing on MEH-PPV. We present our analytical model in which FRET from the polymer to the CTC is considered as dissociation mechanisms of polymer singlet excitons. We analyze the experimental data on PL quenching in MEH-PPV films and solutions using our model. The model takes into account both FRET processes: energy transfer from polymer to the CTC and energy transfer from polymer to another polymer. The model also takes into account previously known general mechanisms of quenching.

Theoretical study of electron transfer in polypyrrole molecular nanowires placed between platinum electrodes

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Over the last decade, the interest in organic materials has significantly increased. It is due to their wide spectrum of use in electronic and microelectronic devices. They are mostly used as a very cheap screens, thin-film tranzistors and photovoltaic cells [1]. The objective of this work is to obtain complex information about the interface between Pt(111) surface and Ppy chain, which could support the present experiments, where Ppy wires are formed via CVD between platinum microelectrodes [2].

The theoretical calculations based on Density Functional Theory (DFT) of the interface between polypyrrole (Ppy) wire and platinum (111) surface will be presented. We perform the total energy calculation of selected structures using fast local-basis set DFT FIREBALL code [3, 4]. Based on these calculations, the electron structure of the studied Pt(111)-Ppy interface was obtained, especially the mechanism of charge transfer over this interface through projected density of states (PDOS). The study of the electron transport and I/V-characteristics was calculated via the Green function method [5] for selected configurations of studied systems.

Surface modification of thin organic layers using the photo-Fries reaction

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As demonstrated in previous works [1] the photo-Fries reaction can be applied to modify the surface properties of thin organic films. In this photoreaction of aromatic esters a rearrangement of the acyl group occurs which leads to the formation of the corresponding o- and p-hydroxyphenone. In this work, polynorbornenes bearing aromatic ester groups in the side chain were synthesized. Thin films of these materials were prepared and irradiated with polychromatic UV light. Ellipsometric measurements showed a large increase of the refractive index (between 0.03 and 0.07) as a result of the photoreaction. The surface properties of the polymer films were characterised by ellipsometry, FTIR and contact angle measurements. The generation of OH groups by UV illumination increased the surface polarity. We found differences in the crystal structure of para-hexaphenyl (PHP) prepared by hot wall epitaxy on illuminated and non-illuminated surfaces of the polymer. The grown PHP structures were characterized by AFM and XRD measurements. In another approach it is shown that the OH groups can be used for a selective immobilization of functional molecules (e.g. fluorescent dyes) in the irradiated zones of the surface.

The same photochemistry was subsequently applied to self assembled monolayers (SAM) on inorganic surfaces which allows the selected modification in ultrathin films. We present the synthesis of the photoreactive trichlorosilanes 12-trichlorosilyldodecanoic acid, phenyl ester (1), and acetic acid, 4-(2-trichlorosilylethyl)phenyl ester (2). We obtained monolayers with compound 1, while compound 2 formed a layer with a thickness corresponding to a bilayer. The surface structures and lithographic patterns were investigated by friction force AFM, XPS, FTIR, XRR and contact angle measurements.

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Self assembled monolayers: A study of 11-mercaptoundecanoic acid on Au – surfaces

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Alkanethiols on gold surfaces serve as a model system of self assembled monolayers (SAMs), as they form well ordered structures due to the strong S-Au-bond.

In the present study, SAMs of 11-mercaptoundecanoic acid (11-MUA) on Au – surfaces were investigated. The acid end group can easily be replaced by other functionalized groups for further studies. SAMs of 11-MUA grown on different substrates were compared. Therefore we investigated amorphous gold on glass, crystallized gold on mica and recrystallized gold foils. A properly cleaned surface is an essential precondition for the growth of well ordered monolayers. We performed chemical cleaning using piranha solution, which is the most common procedure, and cleaning in a UHV – chamber by Ar - sputtering.

We used two different methods to prepare the SAM: SAM formation ex situ in solution is the common practice due to the easiness of this method. However, when preparing the SAM by physical vapour deposition in a UHV chamber, one profits from well defined conditions and exclusion of the influence of the air.

A plenty of methods were used to characterize the SAM of 11-MUA on the respective Au - surface. The presence of 11-MUA on the surface could be shown by X-ray photoelectron spectroscopy (XPS). The increase of the contact angle indicates the influence of the hydrophilic acid group. Individual molecular vibrations were demonstrated by IR – spectroscopy, which allows us to investigate the arrangement of the SAM on the substrate. Thermal desorption spectroscopy (TDS) measurements were performed to get information about the stability and the dissociation reaction during heating. Low energy electron diffraction (LEED) was used to determine the structural arrangement of the SAM. Atomic force microscopy (AFM) studies show the surface structure. Furthermore, XRD measurements were performed on the solid 11-MUA to get information about the crystalline structure of the solid material.

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The Effect of Self-Assembled Monolayers on the Mobility and Contact Resistance in Polymer FETS

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We have investigated charge carrier injection into two semiconducting polymers in field-effect transistors. Self-assembled monolayers (SAMs) of alkanethiols and perfluorinated alkanethiols are used to tune the work function of the gold source and drain electrodes in this device.

The presence of an interfacial dipole associated with the molecular monolayer at the metal-semiconductor interface changes the work function of the electrodes, and, hence, the injection of the charge carriers.

The FET characteristics are analyzed with the transfer line method (TLM). By using this method we have found the mobility for poly(2-methoxy-5-(2'-ethylhexyloxy)-1,4-phenylene vinylene) (MEH-PPV, $\mu_{\text{FET}} = 4 \times 10^{-4} \text{ cm}^2\text{V}^{-1}\text{S}^{-1}$) and for regio-regular poly(3-hexyl)thiophene (P3HT, $\mu_{\text{FET}} = 1\text{-}2 \times 10^{-2} \text{ cm}^2\text{V}^{-1}\text{S}^{-1}$). The contact resistances extracted from the TLM are at least one order of magnitude larger for the SAM-modified gold contacts with respect to the untreated contacts.

Hole injection barrier optimization at ITO/organic interfaces modified with strong molecular acceptors

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The hole injection barriers at interfaces between N,N'-diphenyl-N,N'-bis(1-naphthyl)-1-1'-biphenyl-4,4''diamine (alpha-NPD) and chemically modified ITO substrates have been studied by ultraviolet photoelectron spectroscopy (UPS). A decreased hole injection barrier was achieved by an appropriate arrangement of oriented dipoles, formed by chemisorption of strong electron acceptors, i.e., tetrafluoro-tetracyanoquinodimethane (F4-TCNQ) or hexacyano-hexaazatriphenylene [HAT-(CN)]. In both cases thin acceptor layers induce coverage dependent work function shifts of more than 1 eV, thereby modifying the barrier to hole injection into alpha-NPD by up to 0.4 eV. We observed a linear dependence of the hole injection barrier versus the work function of modified ITO substrates. However, the electron transfer creates localized states at the interface which may represent centers for Fermi level pinning at these interfaces. We find constant hole injection barriers for substrate work functions greater than 5.1 eV.

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Adsorption of 1,4,5,8,9,12-Hexaaza-triphenylene-2,3,6,7,10,11-hexacarbonitrile on Cu, Ag, and Au

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Deposition of particularly electron poor organic molecules on the surface of high work function metals, such as copper, silver, or gold, provides an efficient way to tune hole-injection barriers in state of the art opto-electronic devices over a wide range. Understanding such interfaces is therefore a crucial task, which can be pursued efficiently combining theoretical and experimental techniques.

The title compound (HATCN) serves as model system for this application. Density functional theory (DFT) calculations in gas phase predict a high electron affinity, thus identifying this molecule as a potential candidate for modifying hole-injection contacts.

Experimental investigations using ultraviolet photoelectron spectroscopy (UPS) show a strong increase of the metal work function when brought onto the (111) surfaces of Cu (0.97 eV) or Ag (0.55 eV) , but a small decrease (-0.37 eV) when adsorbed onto Au(111). DFT based band structure calculations were employed to rationalize these work function modification differences theoretically. We find that upon adsorption, severe geometric changes take place compared to the gas phase structure. Beside other effects, a slight bending of HATCN is predicted, in close analogy to the strong electron acceptor F4TCNQ. By variation of the starting geometry in the calculations, the influence of the docking site on the binding energy is investigated. By projecting the electron density on spherical harmonic functions located on each HATCN atom, the projected density of states (PDOS) is obtained and compared to UPS spectra.

Packing density and alignment of the molecules on Ag was experimentally investigated using scanning tunnel microscopy (STM), yielding hexagonal patterns. On the basis of the Tersoff - Hamann approach, a detailed STM-image was simulated (using the DFT-based electronic structure) and compared to the experimental results.

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Theoretical and Experimental studies of Anthraceneselenol SAMs on Au(111)

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Due to their promising electronic properties aromatic molecular materials have attracted significant interest in connection with potential applications in the field of molecular and organic electronics. Of particular interest are interfaces between such organic films and metal substrates because they dictate charge injection properties. Self-assembled monolayers (SAMs) of fully conjugated molecules offer a considerable conductivity and thus provide an interesting class of model systems to study in depth the structure of such interfaces on a molecular level. In the present study various experimental techniques (including STM, LEED and UPS) were combined with density functional theory based slab-type band-structure calculations to derive structural and electronic properties for the case of anthracene-2-selenol SAMs on Au(111). From these calculations valuable details about the charge rearrangements at the surface, binding energy, work function modification upon SAM formation, as well as the alignment between molecular levels and metallic states can be derived. Of prime importance to this contribution is a detailed microstructural characterisation, where we use the calculations to highlight potential pitfalls in the interpretation of STM pictures of aromatic SAMs.

Tuning of the interchain interaction and the photovoltaic performance in polymer-polymer blends

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Organic solar cells fabricated from conjugated polymers attracted increasing attention due to the ability of low-cost manufacturing. A challenge in photovoltaic devices is to achieve efficient charge separation of bound electron-hole pairs formed after photoexcitation. By blending two conjugated polymers with different HOMO and LUMO energies together, a bulk heterojunction (BHJ) forms and the interface area in the film increased dramatically. Therefore, the possibility for excitons to reach the BHJ and to dissociate is largely enhanced.

It is reported that the types of solvent used for spin coating, the spin coating conditions (speed, temperature, concentration...) as well as the different solubility of the two components in the chosen solvent have a significant influence on the polymer blend morphology [1-3].

We have compared M3EH-PPV:CN-Ether-PPV blends prepared from three different solutions with respect to photoluminescence, morphology and solar cell performance. A fill factor (FF) of 44% and an energy conversion efficiency of 1.4% was achieved for devices made from a Trichlorobenzene (TCB) : chloroform (CF) solvent mixture. This fill factor is significant higher than the 35% obtained from previous studies on the same polymer blend but prepared from chlorobenzene [4]. The improved FF in the mixed solvent is not caused by increased charge carrier mobility as confirmed by the photoinduced-charge-extraction-by-linearly-increasing-voltage technique (Photo-CELIV) [5,6] measurements. Instead, an anticorrelation between the FF and the photoluminescence emission from a charge-transfer state (exciplex) was found. We attribute the increased FF to the more efficient free charge carrier generation, which is the limiting factor for the solar cell performance in this system.

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Plasma polymerization mechanisms study: from the gas phase to the surface

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Nowadays several processes are used to deposit organic coating on surfaces such as Plasma-Enhanced Chemical Vapour Deposition (PECVD), spin coating, deep coating. Amongst those, the plasma polymerization (PP) offers many advantages: it is a green process producing plasma polymer films that can be homogeneous, pinhole-free and tightly adherent to their substrates. Furthermore thickness, morphology and stability of the layer can be adapted by tuning plasma parameters (pressure, input power, monomer flow rate, duty cycle...).

Up to now, PP is a very empirical process and only some few fundamental studies have been carried out. The goal of our study is to establish some correlations between the plasma gas phase and the chemical composition and morphology of the polymer deposited film. On one hand plasma will be characterized by mean of mass spectrometry and optical emission spectroscopy, in order to analyse the discharge ; on the other hand, the organic layer will be analysed by X-Ray Photoelectron Spectroscopy (XPS) and Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS). In particular, this latter technique was newly improved in our lab to provide molecular information during dynamic depth-profiling of polymer layers. This will allow us to acquire a better understanding of the PP process.

Investigation and modeling of the dielectric/semiconductor interface properties in organic field-effect transistors

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The interface between an organic semiconductor and a dielectric layer plays a key role in the performance of the Organic Thin-Film Transistors (OTFTs)[1] because the charge carriers flow inside the first few nanometers in the channel. Therefore, engineering an interface that promotes synergistic interactions between the semiconductor and dielectric is essential in achieving optimum FET performance. Recently, many studies on this interface [1,2] have been published showing that it is still controversial which are the precise phenomena that rule charge transport at this interface; this is especially true for electrons. Therefore further investigation is still due.

In this work we aim at contributing to the picture of the charge trapping, charge transport and the defects at the interface by means of either Capacitance-Voltage measurements with varying the frequency on Metal-Insulator-Semiconductor (MIS) structures and I_{ds} - V_{ds} / I_{ds} - V_{gs} characterization on OTFTs devices. Moreover, photocurrent and electrochemical impedance spectroscopy characterization have been employed to give more information about the nature of the trap states for both electrons and holes at the interface between dielectric and semiconductor.

Different organic dielectric materials have been employed as an insulating layer for MIS and FET structures, namely PVA, PVA with Ammonium Dichromate, PVP, polydimethylsiloxane (PDMS) and polymethylsilsequioxane (pMSSQ). Both pentacene and sexithiophene have been employed as semiconducting layer. Semiconductor films were grown simultaneously both on MIS and OTFTs in the same environmental conditions.

Significative differences of electrical parameters as threshold voltage and hysteresis have been measured in transistors which have as dielectric layer a thin PVA film when a cross-linking agent for this polymeric dielectric (Ammonium Dichromate) has been added during assembly. . This aspect, still under study, is particularly interesting as it suggests the possibility of playing with the composition of the dielectric layer for modulating interface properties.

First results on a transistor model that includes traps action in the channel will be shown and used to fit experimental results.

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Morphology and OFET properties of poly(3,3''-didodecyl-[2,2':5',2'':5'',2''']-quaterthiophene) (PQT-12) with different molecular weights

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It is well-known that molecular packing in thin-film organic field-effect transistors plays a crucial role in determining their field-effect mobilities. Here, we used poly(3,3''-didodecyl-[2,2':5',2'':5'',2''']-quaterthiophene) (PQT-12), which tend to adopt a better planar conformation compared to well-known poly(3-hexylthiophene) (P3HT). Since it is well established for P3HT that the average chain length largely determines the OFET-properties [1,2], we investigated different molecular weight fractions of PQT-12 ($M_w = 1,700$ to $26,500$ g/mol) regarding to morphology and transport. In contrast to findings on P3HT, the OFET mobilities were above 0.001 cm²/Vs also for the lowest molecular weight fraction and the smallest mobility (10^{-5} cm²/Vs) was found in the intermediate molecular weight fraction. Studies of the optical, thermal and structural properties of PQT-12 solid samples suggest that the fraction with the shortest chains forms highly-crystalline layers. We attribute this behaviour to the very narrow molecular weight distribution of this low molecular weight fraction. Apparently, the OFET properties of both PQT-12 and P3HT are similar in that the OFET mobility depends largely on the overall crystallinity of the semiconducting layer.

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AFM and PEEM Study of the in-situ Growth of 6P on TiO₂ (110) and Cu (110) in UHV

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The controlled in-situ deposition of 6P onto the (110) surfaces of TiO₂ and Cu in UHV allows the growth of 6P needles and 6P islands to be monitored in real time by Photo Emission Electron Microscopy. In this manner, growth parameters, as a function of crystallographic direction, can be determined and can explain the highly anisotropic growth of needles of lying down 6P molecules.

Spot analysis of specific areas on the surface, by photo-emission, allow differences to the local workfunction that arise during 2nd and 3rd layer growth of the islands of standing 6P molecules to be measured.

Furthermore, high resolution Atomic Force Microscopy images acquired for the same surfaces in UHV reveal the true morphology of the needles of 6P to be that of extended bunches of smaller needles that have an integer width that is pre-determined by the underlying substrate. In conclusion, it is shown that the combination of AFM and PEEM in UHV are useful due to the extent of the combined measurement scale from 1 nm to 120 μ m.

In addition, these techniques are complementary due to the z-height sensitivity of the AFM and the ability to probe the electronic structure by PEEM.

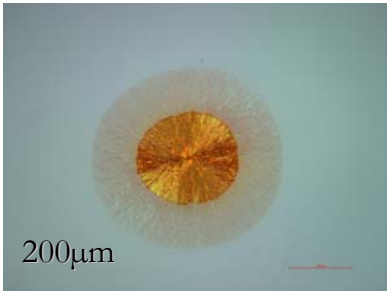
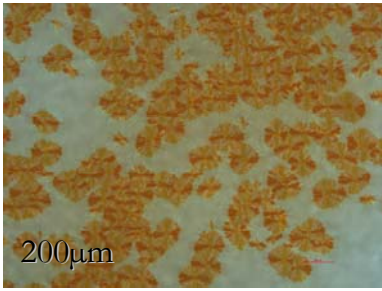
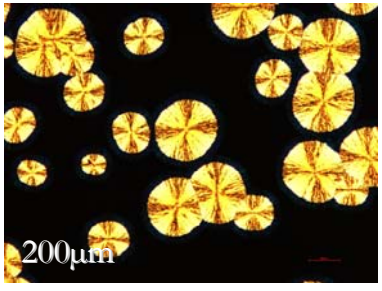
Rubrene thin film characteristics on Mica Substrate

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In the last decades, significant progress has been made in the field of organic electronics. Among the different materials, Rubrene, a derivative of tetracene with phenyl substituents attached to the side of the tetracene backbone, has recently gained much interest. In addition, it exhibits one of the highest reported electronic mobilities at room temperature observed in field effect transistor devices ($20 \text{ cm}^2/\text{V.s}$)[1]. However, this high mobility was obtained only in single crystalline bulk material. The big challenge is to demonstrate similar results in thin films of rubrene. Rubrene films have been evaporated on mica, natural $\text{SiO}_2/\text{n+Si}$ (111) and sapphire (10-10) substrates by using Hot Wall Epitaxy. To optimise the growth conditions, the deposition rate, the substrate temperature and the growth time were changed systematically. AFM, SEM and polarized optical microscope techniques have been used to characterize the grown rubrene thin films. As observed in the optical microscope the thin films show three regions: i) crystalline discs, ii) an unknown ring shaped structure around the centre of the crystalline discs and iii) a matrix, which is supposed to be amorphous. The discs of lamellar structure have a similar shape as reported in the literatures [2,3]. The same structures have been found for rubrene films on different substrates. The size and the density of the disc shaped islands could be controlled by the deposition rate, the substrate temperature and the growth time. The optical absorbance spectra of the rubrene films were measured and compared with spectra for single crystalline rubrene and the molecule in solution [4]. The future work will be concentrated on making transistor out of these crystalline rubrene discs.

| Tsub=90°C | Tsource =235°C | Twall =235°C | Growth time=1h |
|---|---|---|----------------|
| R/mica | R/sapphire | R/Si(n+) | |
|  |  |  | |

Fig(1):Rubrene grown on mica, sapphire and Si(n+) by HWE.

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Modelling of charge carrier transport in semiconductors and semiconductor devices

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This contribution is meant to give an overview of our work that is concerned with the development and application of kinetic theory-based methods to describe the charge carrier transport in bulk semiconductors and semiconductor devices at the mesoscopic scale. By employing transport models that include (but are not limited to) drift-diffusion- as well as semi-classical (Boltzmann and Wigner equations) approaches, the dynamics of the electrical potential, the charge carrier distribution across the entire device (or components thereof), as well as the dynamics of the associated properties can be *deterministically* predicted.

One major challenge is to clarify the transport mechanism and the associated carrier-phonon interaction in a given bulk material, since, particularly if we deal with organic or hybrid organic-inorganic materials, hopping-, or band-transport, or a superposition of both needs to be anticipated. As an associated task, we adapt the methodology, that has been successfully implemented for inorganic materials already, to account for the peculiarities of the predominant transport regime.

Moreover, the consideration of the actual geometry or device set-up allows us to elucidate not only “intrinsic”, i.e., bulk-related effects, but also aspects that arise due to structuring of the material (e.g., quantum confinement) or due to the formation of interfaces, such as contacts or heterojunctions.

We will illustrate the impact of the aforementioned factors with the help of examples in which we investigate the transport dynamics related to electron-phonon scattering in semiconductors and carbon-nanotubes with a recent extension to kinetic studies on graphene sheets. Furthermore, certain aspects that are specifically related to transport simulation in organic semiconductors will be discussed (for a more detailed description, see also contribution of S. Possanner et al.).

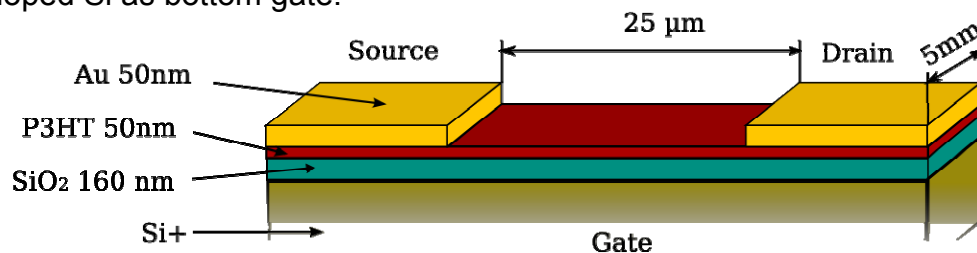
Charge transport in organic semiconductors: commonly used models and comparison to temperature dependent measurements in organic thin film transistors:

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Temperature dependent measurements are the most important technique to determine the model for charge transport in organic semiconductors. The commonly used models found in the literature are briefly summarized. They include: the Bässler model, the multiple trapping and release model, and the percolation model. We fit the temperature dependence of various device and materials parameters obtained from each of these models to measured values from cryogenic and heating experiments on poly(3-hexylthiophene) (P3HT) based thin film transistors. Charge carrier mobility, threshold voltage, and dependencies on charge density in the channel and contact resistance will be discussed.

The investigated transistors consist of top source and drain gold contacts evaporated through a shadow mask on spin coated P3HT film with 150nm SiO₂ as dielectric and highly doped Si as bottom gate.



Influencing the growth of Pentacene with Langmuir Blodgett films

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The Langmuir-Blodgett technology allows the fabrication of ultra thin, highly ordered organic films. A molecular monolayer spread at the air-water interface is transferred onto a solid substrate. This process can be repeated several times with the same substrate to form multilayer films. The layers influence the growth of pentacene by means of different grain sizes and orientation of the molecules. We hope to be able to use this effect to improve the characteristics of organic field effect transistors.

In our experiments, we deposited several layers of pentacosanoic acid (diacetylene) on top of silicon oxide substrates with different surface pre-treatments. Perfluorinated self assembled monolayers, and hexamethyldisilazane (HMDS) make the surface hydrophobic, whereas plasma etching makes it hydrophilic. These modifications were mainly meant to influence the wettability of the silicon oxide. It is very important for the application of LB-films and was quantified by contact-angle measurements. The LB-films were applied in varying number of layers on the different substrates. Their characterization was done by ellipsometry, X-ray reflectivity and atomic force microscopy. Pentacene was grown on top of the LB-layers by vapor deposition and thereafter imaged by AFM. From these samples FETs were built by evaporating gold contacts on top. The results of the experiments will be presented in this contribution.

Current density variations near the metal-semiconductor transition

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The spatial and temporal variations of the current densities that flow in thin films are related to the underlying electronic transport mechanisms. When the electronic states are delocalized, as they are in a metal, the variations tend to be small. Larger variations are expected in a film where the electronic states are localized such as a hopping conductor. The goal of this project is to make direct measurements of the variations in space and fluctuations in time of the electrostatic potential and current densities in a variety of materials that are near the transition between metallic conduction and hopping conduction. This is particularly relevant in molecular crystals and organic conductors where the conductivity is thermally activated. In these films, variations in the characteristics are often observed from device to device. There are theoretical indications that large variations should be observed within a single device but there are not sufficient measurements to test this prediction. To measure the variations in the surface potential as a function of position, Kelvin Probe Force Microscopy (KPFM) and Electrostatic Force Microscopy (EFM) will be used. These are noncontact techniques that measure the electrostatic forces between the surface and a conducting atomic force microscope tip. We will also measure the potential directly by putting a Scanning Tunneling Microscope (STM) tip in direct contact with the films. This method has better spatial resolution than KPFM. The STM measurement will be made with a micromanipulator system. Using this system, up to six STM tips can be brought into contact with the sample simultaneously. The micromanipulator system can be operated inside a scanning electron microscope so that the relative positions of the STM tips can be observed. In a typical measurement, a voltage is applied between two stationary tips while the voltage as a function of position is measured with a third tip. Since the tips can be placed a few microns from each other, electron transport at high electric fields can be investigated without applying very high voltages. The high electric field regime is the most relevant for transistor applications.

Performance Improvement of Dye-Sensitized Solar Cells based on Multi-Walled Carbon Nanotube Composite Materials

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Dye-sensitized solar cells (DSSCs) are in the spotlight of the light harvesting devices owing to the low production cost, simple fabrication processes, environmental compatibility, as well as the comparable energy conversion efficacy with the amorphous silicon solar cell. Many attempts have been reported to improve the efficiency and long term stability by the incorporation of carbon nanotubes (CNTs) into the front electrode, for example, by chemical vapour deposition (CVD) or by CNTs functionalized with titanium dioxide (TiO_2). However, to the best of our knowledge, no report mention about the benefit of the platinum (Pt)-CNT composite as the back electrode material.

We report a simple, novel method for improving the DSSC energy conversion efficiency by the addition of multi-walled carbon nanotubes (MWCNTs) into the TiO_2 active layer and the Pt catalytic film. The J - V characteristic of the as-prepared DSSCs with an active area of 0.36 cm^2 was measured under the air mass 1.5 illumination standard. Compared with the conventional DSSCs, the incorporation of MWCNTs into either the front or the counter electrodes was found to increase on average the energy conversion efficiency by approximately 1.2 and 1.9 times, respectively. Interestingly, the addition of MWCNTs into both electrodes in a single DSSC boosted the solar cell performance by 2.3 times. Two mechanisms may be responsible for this efficiency enhancement: the improved conductivity of the films from the CNT additives in the case of the TiO_2 electrodes and an increase in the surface area. However, with CNT additives of higher than 1% by weight in the electrodes, the conversion efficiency decreases gradually. This seems to result from a poor optical transparency of the composite films.

Keywords: dye-sensitized solar cells; carbon nanotubes; platinum

Universal Arrhenius temperature activated charge transport in diodes from disordered organic semiconductors

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Charge transport models developed for disordered organic semiconductors predict a non-Arrhenius temperature dependence $\ln(\mu) \propto 1/T^2$ for the mobility μ . We demonstrate that in space-charge limited diodes the hole mobility (μ_h) of a large variety of organic semiconductors shows an universal Arrhenius temperature dependence $\mu_h(T) = \mu_0 \exp(-\Delta/kT)$ at low fields, due to the presence of extrinsic carriers from the Ohmic contact. The transport in a range of organic semiconductors, with a variation in room temperature mobility of more than six orders of magnitude, is characterized by an universal mobility μ_0 of 30-40 cm²/Vs. As a result we can predict the full temperature dependence of their charge transport properties with only the mobility at one temperature known.

Integrated organic sensor modules

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In this poster we present the integration of different optical, optoelectronic and electronic devices into one organic sensor module. The sensor's working principle is based on luminescence quantum-yield changes of chromophores upon interaction with respective gases (i.e. oxygen). Integrateable light sources and detectors (organic light emitting devices and organic photodiodes) are developed to match the fluorescence excitation and emission characteristics of the sensor molecules. These building blocks are the core elements for the integration into one sensor device, together with optical elements (i.e. waveguides). This integration strategy requires a variety of optical, optoelectronic and electronic interfaces. The characterisation and tailoring of such interfaces in the nanometer range are crucial to achieve the required performance and a high reliability of the complete integrated sensor system.

Pentacene and para-sexiphenyl heterostructures on clean and oxygen reconstructed copper surfaces

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Modern organic semiconducting devices consist of a multiplicity of organic layers but detailed crystal growth studies of these heterostructures are scarce. The results presented in the present study are twofold: first the orientation and crystal growth of pentacene on Cu(110) and on the oxygen reconstructed Cu(110)-p(2x1)O (CuO) surface are shown followed by the growth of para-sexiphenyl (6P) on the respective pentacene layers. The growth of pentacene on the two different substrates are interesting on its own, as they are able to orient rod-like molecules due to their pronounced surface corrugations in perpendicular directions. Indeed an alignment of the long molecular axis parallel to the close packed CuO rows ([001] direction) is seen for the CuO surface. On the other hand, for the pristine Cu surface the long molecular axis is rotated by $\pm 5.5^\circ$ from the close packed Cu rows ([1-10] direction). This misalignment can be understood since the long molecular axis is exactly off by this 5.5° from the long axis of the pentacene surface unit cell and therefore this particular growth seems to be dominated by the alignment of copper and pentacene crystal directions rather than molecular alignment. Despite these differences pentacene grows with the (022) net plane parallel to the surface on both substrates.

To complete the heterostructure, 6P is evaporated on top of the pentacene layers and the epitaxial relationships between the layers of the two heterostructures are found to be the same. In other words, the different alignment of the 6P layers can be traced back to the different alignments of the underlying pentacene organic layers. In both cases 6P molecules with (20-3) net planes parallel to the surface grow. The in-plane orientation of the heteroepitaxy (6P on pentacene) is seen to be dominated by the alignment of crystal directions rather than molecular alignment.

All-organic magnetic molecules: synthesis, magnetic properties, and thin film growth

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In the frame of the research on organic semiconductors, the growth of thin films is necessary to integrate the new materials in devices. In order to control their solid state properties, it is of primary importance to drive the growth of thin films and several tools are available: among them, the use of external magnetic fields has been demonstrated to be effective, even in the case of diamagnetic aromatic molecules [1]. The availability of paramagnetic molecular semiconductors would give the opportunity to better exploit the use of magnetic fields during the film growth [2]. Moreover, the availability of a magnetic semiconductor could allow to observe new phenomena and to apply them in devices, e.g. in the field of spintronics or gas sensors.

Here, we present the synthesis and characterization of new organic semiconductors, where a conjugated backbone is joint with paramagnetic substituents. The two examples discussed here (compounds **2** and **4** in Fig. 1) were prepared by reacting a tetra-fluoroacridine (compounds **1** and **3** in Fig. 1) with the TEMPO free radical. Solution electron paramagnetic resonance (EPR) spectroscopy was used to assess the number of radical centres per acridine unit.

Magnetic characterization was carried out on the poly-crystalline powder by collecting magnetization curves as a function of both magnetic field intensity and temperature. After subtracting the diamagnetic contribution of the molecule using the Pascal coefficient, a paramagnetic behavior was observed, as shown in Fig. 2. Best fit of the experimental data gave a value $\mu_{\text{eff}} = 1.73 \mu_B$ in complete agreement with what expected for a single spin. Also effects related to the presence of ferromagnetic and antiferromagnetic correlations will be discussed.

Finally, thin films (from 10 to 20 nm-thick) of these molecules were grown by Organic Molecular Beam Epitaxy on different substrates and under different conditions, then their morphology studied by Atomic Force Microscopy. The growth proceeds following an island mode and a higher island density was found when deposition is carried out under a magnetic field.

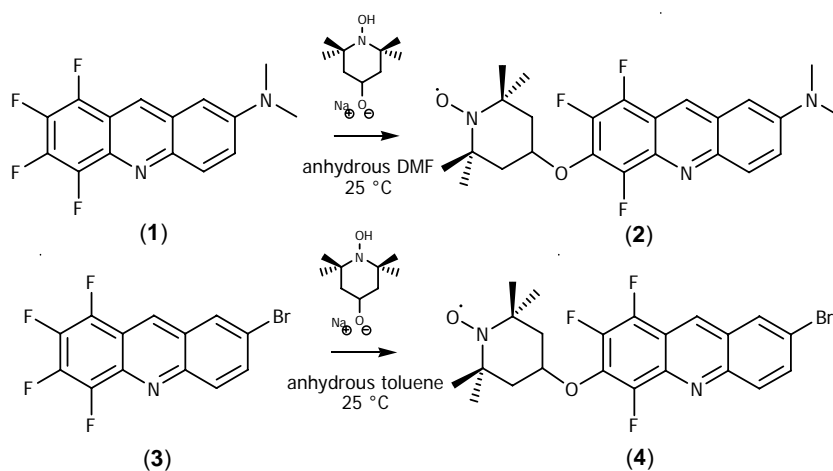


Figure 1 – Scheme of the synthetic route to the paramagnetic compounds based on tetrafluoroacridine.

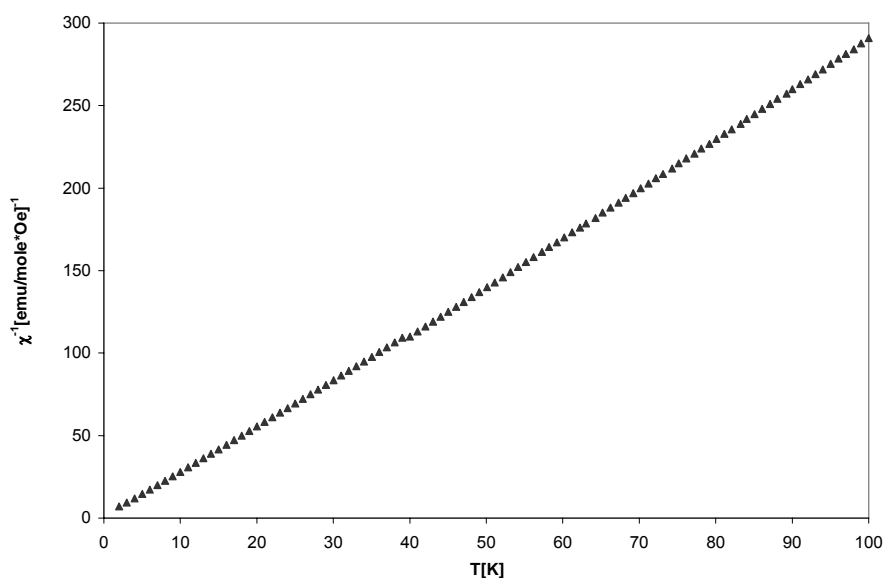


Figure 2 – Inverse magnetic susceptibility of compound **2** as a function of temperature, as deduced after correction for the experimental diamagnetic contribution.

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Material optimization for light emitting diodes

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There is a need for improvement of the material properties for organic polymer LEDs. We look for fundamental issues concerning blue emitting polymers. The aim of this study is to find the relation between chemical structure and device properties.

Materials for Organic Bulk Heterojunction Solar Cells and Sensor Applications

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We discuss the synthetic routes towards the large scale synthesis of two materials that have shown promising efficiencies in bulk heterojunction solar cells. Apart from application in scientific research, these materials will also be optimized for inkjet printing and large scale processing, for example for use in sensor devices based on organic electronics.

Flexible Organic LEDs for Lighting and Signage

S. Harkema

Holst Centre (NL)

The Holst Centre is an independent R&D institute that develops generic technologies and technology platforms for autonomous wireless transducer solutions and systems-in-foil. A key feature of the Centre is interaction and cooperation with industry and academia. It is this kind of cross-fertilization that will enable the Holst Centre to tune its scientific strategy to industrial needs.

Intensive cooperation in an open innovation spirit is essential for successful long-term, cost-effective research and future product innovation. Interaction and cooperation with both academia and the industry, including small- and medium-sized enterprises, enables the Holst Centre to tune its scientific strategy to the long-term corporate product strategies of its partners. A beneficial transfer of technology to the industry is guaranteed and market requirements can be anticipated.

Research at the Holst Centre is structured in two strategic program lines: the 'wireless autonomous transducer solutions' program line and the 'system-in-foil products and production' program line. The expertise of both IMEC and TNO will be combined in the two strategic program lines.

The poster that will be presented concerns System-in-foil products and production. Printing electronics on thin substrates such as foil will create a revolution in the electronics industry, enabling ultra light and ultra thin, flexible, easy-to-wear electronic products such as lighting and signage devices, reusable and disposable sensor devices, foldable solar panels and displays. Production processes such as now used in the paper printing industry will enable to make these devices in large sizes and quantities at low costs.