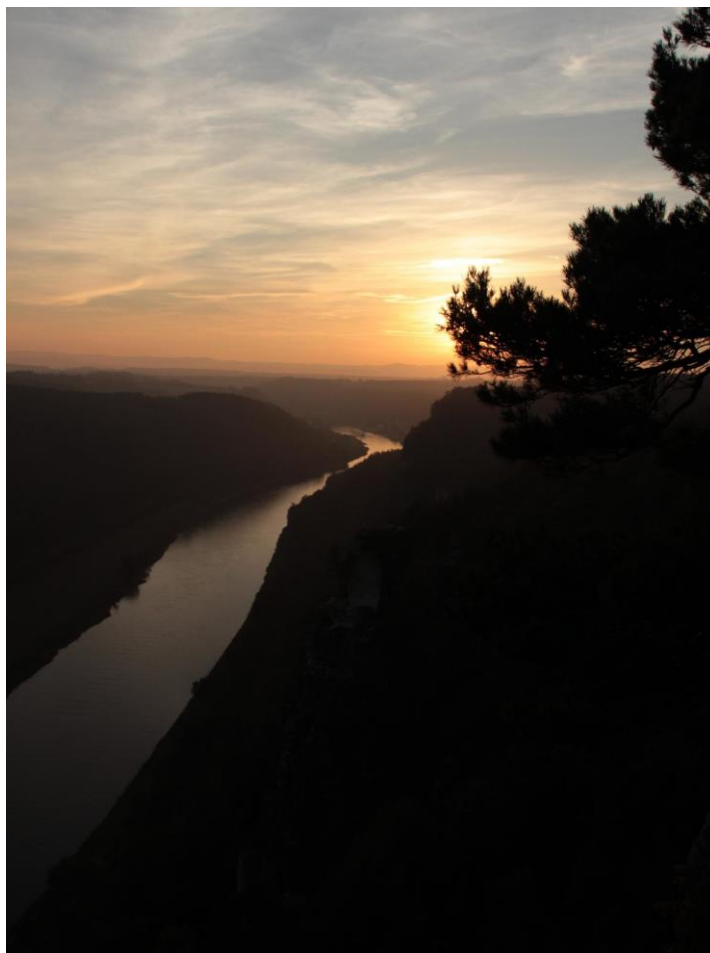


IHRS NANO NET Annual Workshop 2015

30 September – 02 October 2015
Berghotel Bastei, Germany



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Venue and organization

Venue

Berghotel Bastei
01847 Lohmen, Germany
Phone: +49 35024 779-0, Fax. -481
E-mail: info@bastei-berghotel.de
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Organization

International Helmholtz Research School for Nanoelectronic Networks (IHRS NANONET)
Helmholtz-Zentrum Dresden-Rossendorf
Bautzner Landstraße 400, 01328 Dresden, Germany
Phone: +49 351 260 3121
E-mail: nanonet@hzdr.de
Homepage: www.ihrs-nanonet.de

Scientific Organizers

Speaker: Dr. Artur Erbe
Institute of Ion Beam Physics and
Materials Research
Helmholtz-Zentrum Dresden-Rossendorf
01328 Dresden, Germany
Phone: +49 351 260 2366
E-mail: a.erbe@hzdr.de

Deputy: Prof. Dr. Gianaurelio Cuniberti
Institute for Materials Science and Max
Bergmann Center of Biomaterials
Dresden University of Technology
01062 Dresden, Germany
Phone: +49 351 463 31414
E-mail: g.cuniberti@tu-dresden.de

Local Organizer

PD Dr. Peter Zahn
Helmholtz-Zentrum Dresden-Rossendorf
Institute of Ion Beam Physics and Materials Research
Bautzner Landstraße 400, 01328 Dresden, Germany
Phone: +49 351 260 3121
E-mail: p.zahn@hzdr.de

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Helmholtz Association (VH-KO-606).**



Agenda

Place: Berghotel Bastei, 01847 Lohmen

updated: 25.09.2015 (PZ)

Wednesday, 30 September 2015

Start	Who	Time (min)	Short Title	Notes
10:30 / 09:45			Transfer from Pirna / Hiking from Wehlen	
12:00			Arrival/Lunch Snacks	
13:00	A. Erbe		Welcome address	
13:15	K. Gothelf	40+5	DNA Programmed Assembly of Polymers and other Molecules	Chair: A. Erbe
14:00	H. Zacharias	40+5	Spin transport through ordered thin films of helical molecules	
14:45		30	Break	
15:15	R. Metzger	40+5	The Smallest Unimolecular Rectifier	Chair: A. Erbe
16:00	T. Huhn	40+5	The Chemistry behind Molecular Electronics	
16:45	all	120	Hiking around Bastei/to Rathen	
19:00			Dinner	

Thursday, 01 October 2015

7:00			Breakfast	
9:00	Lokamani	12+3	Electron transport in Diarylethene Switches	Chair: S. Gemming
9:15	J. Kelling	12+3	Electronic Transport through Au-contacted, Thiol terminated PEEB	
9:30	Y. Aleksandrov	12+3	Electrical detection of ferromagnetic resonance	
9:45	E. Baek	12+3	Si Nanowire FETs	
10:00	D. Deb	12+3	Top-down fabrication and characterization of silicon nanowires	
10:15		30	Break	
10:45	M. Meyyapan (t.b.c.)	30+5	t.b.a.	
11:20	all	60	Annual Meeting	prepare evaluation
12:30			Lunch	
14:00	G. Öktem	12+3	Oligothiophenes	Chair: A. Kiriy
14:15	M. Hetti	12+3	Polymer Functionalized Magnetic	
14:30	B. Iyisan	12+3	Multifunctional and dual-responsive polymersomes	
14:45	J. Nawroth	12+3	Surface Patterning and Positioning of DNA Origami	
15:00	B. Teschome	12+3	Arrangement and characterization of functional DNA origami	
15:15		30	Break	
15:45	E. Scheer	40+5	Atomic and Molecular Switches	Chair: M. Helm
16:40		120	Poster Session	
19:00			Dinner including Poster Prize ceremony	
20:30	Steering Committee + Advisory Board		Meeting	

Friday, 02 October 2015

7:00			Breakfast	
9:30	Check-Out (latest 10:30)			
10:00	A. Keller	30+5	DNA origami nanostructures	Chair: P. Zahn
10:35	D. Ryndyk	30+5	Modeling of molecular nanostructures	
11:10	J. Schuster	30+5	Simulations for present and future nano electronics at Fraunhofer ENAS	
12:00			Lunch	
13:00			Coffee	
13:30	C. Herrmann	50+10	Controlling and understanding conductance in molecular junctions	Chair: A. Erbe
14:30	A. Erbe		Closing	
14:45			Departure	

1) Posters can be mounted on arrival. There is no given order. They should be on display the whole time.

2) Please, remove your poster on Friday at latest 13:30.

Invited Talks

Kurt Vesterager Gothelf

DNA Programmed Assembly of Polymers and other Molecules

Carmen Herrmann

Controlling and understanding conductance in molecular junctions

Thomas Huhn

The Chemistry behind Molecular Electronics

Robert M. Metzger

The Smallest Unimolecular Rectifier

Elke Scheer

Atomic and Molecular Switches

Helmut Zacharias

Spin transport through ordered thin films of helical molecules

Keynote Talks

Adrian Keller

Single-molecule studies of biochemical and biophysical processes using DNA origami nanostructures

Dmitry A. Ryndyk

Modeling of molecular nanostructures on metal and semiconductor surfaces

Jörg Schuster

Simulations for present and future nano electronics at Fraunhofer ENAS

Student Talks

Yuriy Aleksandov

Electrical detection of the ferromagnetic resonance in an individual, nanoscale magnetic stripe

Eunhye Baek

**Optoelectronic Double-Gate Modulation
in Metal Ion-doped Thin Film-coated Si Nanowire FETs**

Dipjyoti Deb

Top-down fabrication and characterization of silicon nanowire reconfigurable field effect transistors with sub 50 nm width

Mimi Hetti

Synthesis and Characterization of Polymer Functionalized Magnetic Nanoparticles for Non-destructive Testing

Banu Iyisan

Multifunctional and dual-responsive polymersomes as smart nanocontainers for biomedical applications

Jeffrey Kelling

Electronic Transport through Au-contacted, Thiol terminated PEEB

Lokamani

**Electron transport in Diarylethene Switches:
A combined theoretical and experimental approach**

Jonas F. Nawroth

Surface Patterning and Positioning of DNA Origami on the Nanoscale

Gözde Öktem

Oligothiophenes as a promising platform for single-molecule nanoelectronics

Bezu Teschome

Arrangement and characterization of functional DNA origami nanostructures for nanoelectronics

DNA Programmed Assembly of Polymers and other Molecules

Kurt Vesterager Gothelf

Center for DNA Nanotechnology (CDNA), iNANO and Department of Chemistry, Aarhus University, 8000 Aarhus C, Denmark.

kvg@chem.au.dk

We are using DNA as a programmable tool for directing the self-assembly of molecules and materials. The unique specificity of DNA interactions and our ability to synthesize artificial functionalized DNA sequences makes it the ideal material for controlling self-assembly and chemical reactions of components attached to DNA sequences. Recently, we applied these methods to DNA templated conjugation of DNA to proteins such as antibodies.[1] In particular we are using DNA origami, large self-assembled DNA structures as a template for positioning of materials such as organic molecules, dendrimers and biomolecules.[2-4] We have also used DNA origami to image chemical reactions with single molecule resolution[4] and to make a 3D DNA origami box with a controllable lid.[5] The main focus of the presentation will be on a recently prepared DNA-phenylene vinylene polymer and its self-assembly on DNA origami for studies of electronic and optical properties (Fig 1).[6]

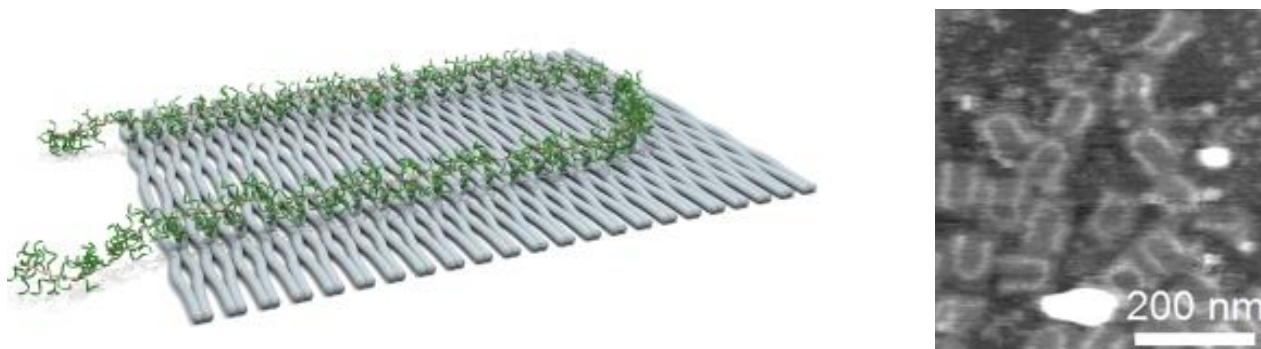


Figure 1. Illustration and AFM image of poly(DNA-phenylene vinylene) on DNA origami.

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- [1] Rosen et al., *Nature Chem.* **6** (2014) 804–809.
- [2] Ravnsbæk; J. B et al., *Angew. Chem. Int. Ed.* **50** (2011) 10851–10854.
- [3] Liu, H. et al., *J. Am. Chem. Soc.* **132** (2010) 18054-18056.
- [4] Voigt, N. V. et al., *Nature Nanotech.* **5** (2010) 200-205.
- [5] Andersen, E. S. et al., *Nature* **459** (2009) 73-76.
- [6] Knudsen, J. B. et al., *Nature Nanotech.* **2015**, doi:10.1038/nnano.2015.190.

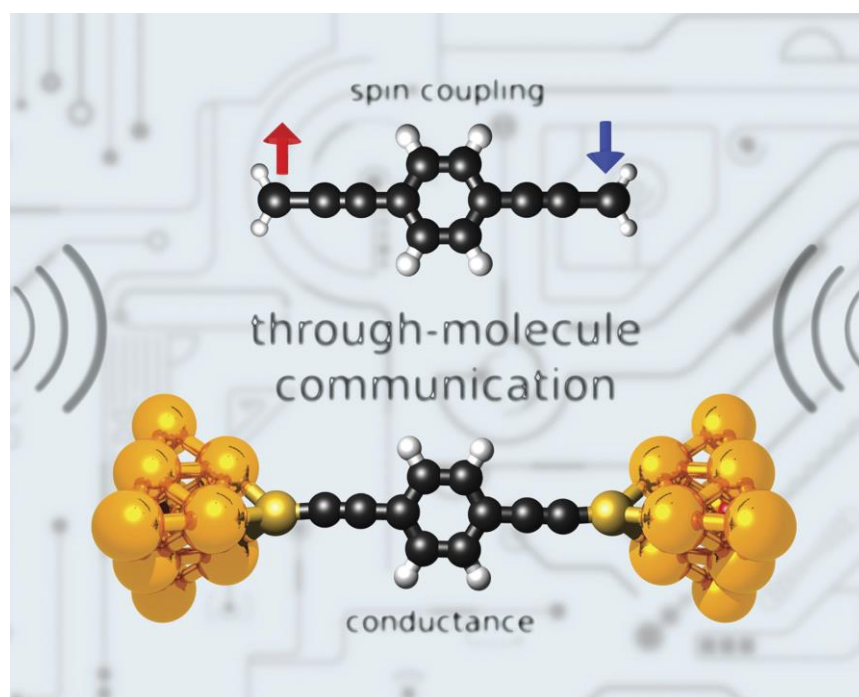
Controlling and understanding conductance in molecular junctions

Carmen Herrmann¹

¹University of Hamburg, Department of Chemistry, Martin-Luther-King-Platz 6, 20146 Hamburg, Germany

Corresponding author: Carmen.herrmann@chemie.uni-hamburg.de

Molecular conductance is measured in different experimental setups such as scanning tunneling microscopes (STMs), molecular break junctions, and nanoparticle arrays. The motivation behind these experiments is not only studying potential reproducible nanoscale building blocks for electronics or spintronics, but also learning about molecules under unusual conditions. We show how theory can help understanding and controlling molecular conductance based on several examples from our research, ranging from a conceptual comparison of conductance and exchange spin coupling, to a study on switching conductance by protonation, to a simulation of combined scanning-tunneling/atomic-force microscopy experiment on platform-mounted porphyrin complexes.



- J. Proppe, C. Herrmann, Communication through molecular bridges: Different bridge orbital trends result in common property trends, *J. Comput. Chem.* **36**, 201 (2015).
- C. Herrmann, J. Elmisz, Electronic Communication through Molecular Bridges, *Chem. Commun.* **49**, 10456 (2013).
- H. Schlicke, C. Herrmann, Controlling molecular conductance: switching off π sites through protonation, *ChemPhysChem* **15**, 4011 (2014).
- N. Hauptmann, L. Groß, K. Buchmann, K. Scheil, C. Schütt, F. Otte, R. Herges, C. Herrmann, R. Berndt, High-conductance surface-anchoring of a mechanically flexible platform-based porphyrin complex, *New J. Phys.* **17**, 013012 (2015).

The Chemistry behind Molecular Electronics

Thomas Huhn¹, Dmytro Sysoiev¹, Mikhail Kabdulov¹,
Fabian Schneider¹, Jannic Wolf¹, Ulrich E. Steiner¹

¹Fachbereich Chemie, Universität Konstanz, 78547 Konstanz, Germany

Corresponding author: Thomas.huhn@uni-konstanz.de

It is well-accepted that molecular electronics is depending on the availability of molecules which offer certain functionalities. A lesser known fact is how much difficulties one might encounter to gain access to those molecules and how sensitive they might be, especially when highly functionalized. In an ideal world molecules would, once they had been prepared, not change their properties and working with them would be pure joy. Unfortunately molecules degrade over time; some are more rapidly than others. Why is that so and what happens to them? And finally, which precautions might help to prevent these processes?

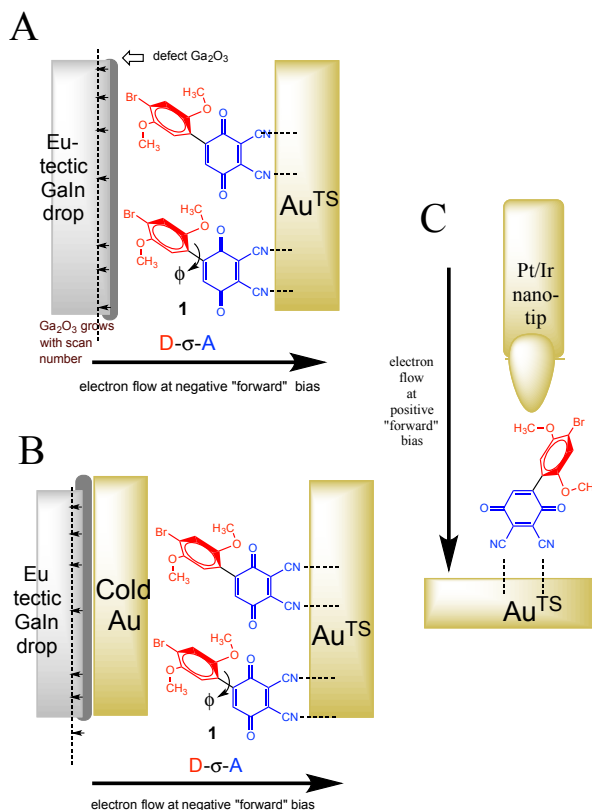
During the first part of my talk I will address those aspects and introduce certain basic concepts of organic chemistry which will prove helpful to identify and possibly avoid the common pitfalls of incompatibilities between molecules and their environment or projected experiments with them. I will illustrate this part of the talk with some of our own examples where the chemistry did not work the way it was initially intended to do and how we finally “worked-around” those problems (or made the best out of it).^[1]

In the second part of my talk I will present some of our new molecules we are currently working on as possible building blocks for a use in molecular electronics in different contact geometries like e.g. molecular break junctions or self-assembled mono-layers.

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(b) J. Wolf, T. Huhn, U. Steiner, *Phys. Chem. Chem. Phys.* **17** (2015) 6066–6075.

The Smallest Unimolecular Rectifier

Joseph E. Meany, Marcus S. Johnson, Stephen A. Woski, and Robert M. Metzger*
 Department of Chemistry, University of Alabama
 Tuscaloosa, AL 35487-0336, USA

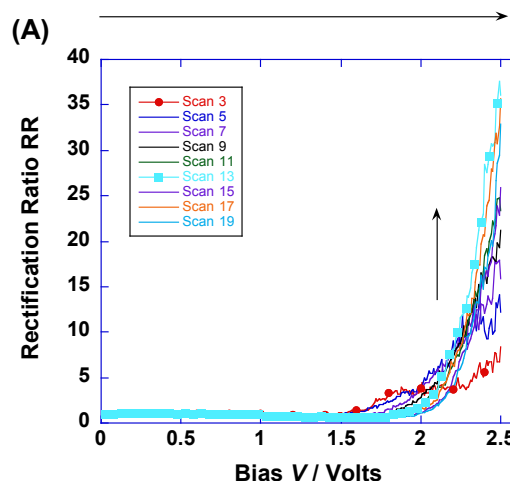
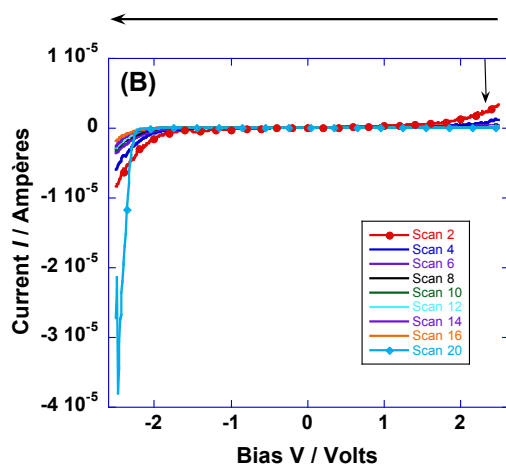


HBQ is a twisted hemibiquinone (weak electron donor + weak electron acceptor with a large intramolecular twist angle $\phi \approx 30^\circ$); it is only 1.1 nm long (by AFM nanodozing).

HBQ chemisorbs onto Au. The DC electrical current is asymmetric, because HBQ rectifies in the "reverse Aviram-Ratner direction".

The rectification ratios are $\text{RR} = 150$ to 200 at 2.5 Volts when studied **(A)** as a monolayer between Au and an eutectic Galn drop; this RR grows upon repeated scans because an interfacial Ga_2O_3 thickens. When instead the **HBQ** monolayer is measured between Au and cold Au **(B)**, (see plots below) RR is smaller, $\text{RR} = 5$ to 40 at 2.5 Volts (but still grows somewhat with scans). When a **single HBQ molecule** is measured

by scanning tunneling spectroscopy **(C)** between Au and a PtIr nanotip, $\text{RR} = 3$ to 8 at 1.5 Volts. HBQ is the smallest rectifier known to date.



Atomic and Molecular Switches

E. Scheer¹, S. Golrokh¹, A. Karimi¹, M. Matt¹, P. Nielaba¹, F. Pauly¹, C. Schirm¹,
M. Valasek², M. Mayor²

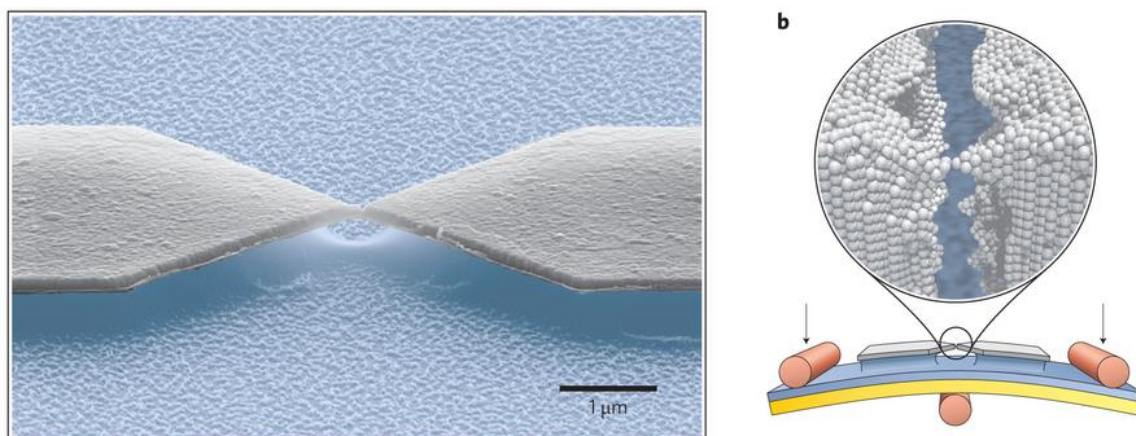
¹Department of Physics, University of Konstanz, D-78457 Konstanz, Germany

²Karlsruhe Institute of Technology (KIT), Germany

Corresponding author: elke.scheer@uni-konstanz.de

Key elements in microelectronics are reliable switches that can be operated as memories. Switches are usually realized by transistors and these components have been miniaturized all the way down close to the atomic scale. However, at such scales three terminals are technically challenging to implement. Therefore alternative control schemes like optical activation of molecules or mechanical drives have been tested.

In this talk I will first present an experiment in which a metallic atomic-size contact has been operated as a reliable and fatigue-resistant two-terminal switch. Current pulses are used to toggle the conductance between two well-defined values in the range of a few conductance quanta. Due to its hysteretic behavior with two distinct states, this two-terminal switch can be used as a non-volatile storage element [1].



At the end I will change gears and will briefly introduce the novel molecular platform of Spirobifluorenes [2] that lends itself for comparative studies of different contacting techniques, i.e. STM and MCBJ. This class represents a tripodal footprint and a conjugated molecular wire that stands upright on surfaces and forms highly-conductive molecular junctions in the MCBJ set-up.

1. C. Schirm et al., Nature Nanotechnol. **8**, 645 (2013)
2. M. Valasek et al., J. Org. Chem. **79**, 7342 (2015), A. Karimi et al., submitted

Spin transport through ordered thin films of helical molecules

H. Zacharias

Center for Soft Nanoscience and Physikalisches Institut, University of Münster, Germany

For spintronic applications the development of a source of spin polarized electrons operating at room temperature is still a challenge. A new approach is based on the interaction of electrons with ordered helical molecules. Early experiments using circularly polarized light to emit photoelectrons from gold surfaces transmitting through monolayers of stearyl lysine [1] and DNA [2] indicated a spin-filtering behavior of such organic layers.

Here we present results on the electron spin polarization observed for various samples of self-assembled monolayers of helical molecules on metal and semiconductor surfaces. Samples are irradiated with circularly and linearly polarized laser radiation at $\lambda = 213$ nm to generate photoelectrons in a single step. The spin of the photoelectrons is analyzed by a Mott polarimeter. Longitudinal spin polarizations of up to about 60% have been measured in case of oligo dsDNA, irrespective of the polarization of the irradiating light [3]. Experiments with chiral membrane proteins and self-assembled monolayers of α -helical oligo-peptides show also spin filtering properties [4, 5]. Similar to DNA a dependence of the spin polarization on the length of the molecules is observed. Recent experiments with enantiomer pure hepta-helicene and for oligo dsDNA covalently bound to Si show promising results.

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e-mail: hzach@uni-muenster.de

Single-molecule studies of biochemical and biophysical processes using DNA origami nanostructures

Adrian Keller

Nanobiomaterials group, Technical and Macromolecular Chemistry, University of Paderborn, Paderborn, Germany

Corresponding author: adrian.keller@uni-paderborn.de

During the last three decades, the field of structural DNA nanotechnology has developed a variety of techniques to assemble DNA into increasingly complex 2D and 3D nanostructures. Nowadays, DNA nanostructures and particularly DNA origami¹ are widely employed in various fields of application such as plasmonics, molecular sensing, and drug delivery.² Due to the great versatility of the DNA origami technique which enables for instance the controlled immobilization of organic dyes, proteins, enzymes, or DNA topologies with nanometer precision, DNA origami substrates can also be employed for the single-molecule study of biochemical and biophysical processes by a variety of spectroscopic and especially microscopic techniques.^{3,4}

In this talk, I will summarize our previous single-molecule investigations of biomolecular damage induced by secondary low-energy electrons. Such low-energy electrons are generated in large quantities during the interaction of high-energy radiation with living matter and represent a major source of biomolecular damage in the cell. Using a novel approach based on atomic force microscopy imaging of DNA origami substrates,⁵ we were able to measure absolute electron damage cross sections for different biochemical species, *i.e.* a single disulfide bond, the B-vitamin biotin, a thymine dinucleotide, and 13-mer oligonucleotides with different sequences. Furthermore, I will outline our current research activities that focus on the application of DNA origami in drug discovery and protein biophysics.

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Modeling of molecular nanostructures on metal and semiconductor surfaces

Thomas Lehmann, Seddigheh Nikipar, Dmitry A. Ryndyk, Gianaurelio Cuniberti

Institute for Materials Science, TU Dresden, Dresden, Germany

Corresponding author: dmitry.ryndyk@nano.tu-dresden.de

The development of molecular electronics during last years showed the growing importance of planar low-dimensional systems. In particular 1D and 2D molecular nanostructures on different surfaces are produced and characterized. Within the NanoNet projects we plan to investigate experimentally and theoretically the properties of molecular wires, which can be grown by on-surface polymerization and investigated by STM in the group of Francesca Moresco (TU Dresden). Ab-initio based theoretical studies will be performed on the adsorption, mechanical and electronic properties of molecular wires on metal and semiconductor surfaces.

The starting point of the theoretical analysis are DFT (Density Functional Theory) and MD (Molecular Dynamics) approaches to calculations of the on-surface diffusion and investigation of possible reaction mechanisms between molecules. In particular we wish to distinguish between covalent bonding and weaker hydrogen bonding. Both mechanisms lead to formation of the ordered structures on the surface, but the covalent bonding is more stable and is required for highly conducting molecular wires. We discuss the methods to find the reaction path and the energy barrier for relevant chemical reactions, in particular the idea and numerical implementation of the Nudged Elastic Band (NEB) method. We pay special attention to possible covalent bonding leading to the polymerization and conjugated molecular structures. Computational design of 1D and 2D structures from monomers and optimization of the monomer properties can be considered as a perspective aim of this research.

The next step is calculation of the electronic properties. First we consider the effects of hybridization between electronic states in the molecules (molecular wires) and the substrate (which can lead to “metallization” of molecular wires). It is important to understand the charge transfer between molecules and conducting substrates. Besides, calculations and analysis of the STM images and STM spectroscopy will be presented. The probing scanning techniques (STM,AFM...) allow the experimental investigation of samples with atomic resolution, and the theoretical model is required able to connect observed images and voltage-current curves with the atomic structure. Finally, we discuss electron transport along molecular wires and functional molecules combined with dangling-bond wires on passivated semiconductor surfaces. The calculation of transport properties is based on the open-source atomistic code CP2K and our home quantum transport code.

Simulations for present and future nano electronics at Fraunhofer ENAS

Florian Fuchs^{2,3,4}, Xiao Hu³, Linda Jäckel¹, Erik Lorenz¹, Jörg Schuster¹,
Fabian Teichert^{2,3}, Christian Wagner^{2,3}, Andreas Zienert³, Hermann Wolf¹

¹Fraunhofer Institute for Electronic Nano Systems (ENAS), Chemnitz, Germany

²Faculty of Natural Science, Technische Universität Chemnitz, Chemnitz, Germany

³Center for Microtechnologies, Technische Universität Chemnitz, Chemnitz, Germany

⁴Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

Corresponding author: joerg.schuster@enas.fraunhofer.de

The simulation group at Fraunhofer ENAS addresses the challenges which come with the shrinking of CMOS-devices to nanoscale dimensions and with the emerging nano-electronic devices based on one-dimensional structures. In close collaboration with the center of microtechnologies, located at Chemnitz University, the group covers state of the art electronic structure and quantum transport simulations for nano-devices. These activities are complemented by the simulation of nanomaterial growth using vapor phase methods. For the latter, atomistic models are combined with continuum models to consider all relevant scales.

ENAS has long standing experience in the field of on-chip interconnects for ULSI CMOS-technologies. Nowadays, further scaling of the on-chip interconnect system is one of the biggest challenges for the further miniaturization of CMOS-technologies. As one example, the in-situ repair of the ultra-low-k dielectrics in the interconnect system was recently simulated by ENAS using quantum chemical approaches [1]. Within the project EVOLVE, ENAS supports the manufacturing of ultrathin diffusion barriers in the interconnect system by simulation based optimization of deposition processes in collaboration with GLOBALFOUNDRIES.

Within the project WAYTOGO FAST driven by the leading european semiconductor companies, the simulation group at ENAS is going to predict the mechanical strain which occurs in transistor channels to be manufactured by future 14 nm FDSOI CMOS technologies. Mechanical strain resulting from the different process steps is crucial for transistor performance and is thus issue of optimization. Computer simulation are the only way to obtain insights how the different strain sources interact within those extremely miniaturized devices.

Nano electronic devices made of quasi one-dimensional structures such as carbon nanotubes or silicon nanowires are promising candidates for numerous applications such as logics, high frequency electronics or sensorics. For a proper simulation of the functionality of those devices a quantum mechanical description is required [2]. However, most of the devices are too big to be covered by electronic structure theory altogether. Thus novel concepts and approaches are required in order to simulate functional nano-electronic devices and its properties [3] as well as the technologies how they are made [4].

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Electrical detection of the ferromagnetic resonance in an individual, nanoscale magnetic stripe

Yuriy Aleksandov^{1,2}, Ciaran Fowley¹, Ewa Kowalska^{1,2}, Alina Deac¹, Jürgen Lindner¹

¹ Helmholtz-Zentrum Dresden - Rossendorf, Institute of Ion Beam Physics and Materials Research, Bautzner Landstraße 400, 01328 Dresden, Germany

² Faculty of Physics, Dresden University of Technology, 01062 Dresden, Germany

Corresponding author: y.aleksandrov@hzdr.de

The radio-frequency magnetization dynamics of nanoscale ferromagnetic materials is of critical importance to applications in spintronics. Electrical detection of the ferromagnetic resonance (FMR) is a powerful technique which has been broadly applied for studying magnetization and spin dynamics of such systems. It has been broadly applied for studying diverse material structures, ranging from ferromagnetic thin films from amorphous [1], single crystal [2], bilayer devices, to a variety of magnetic tunneling junctions (MTJ)[3]. By this highly sensitive method, one can quantitatively determine such as the nonlinear magnetization damping, the phase diagram of the spin-transfer driven dynamics or parametric spin wave excitations and the magnetic anisotropies at work in the system.

Various mechanisms are used as a detection scheme [4], since AMR involves spin rectification it generates a time-averaged dc voltage in magnetic medium via FMR. In this study we have focused on the magnetization dynamics of Permalloy nano-wires with different width and lengths. We observed the variation of modes with the nanowire geometry, edge sharpness.

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Optoelectronic Double-Gate Modulation in Metal Ion-doped Thin Film-coated Si Nanowire FETs

Eunhye Baek¹, Taiuk Rim², Larysa Baraban¹, Gianaurelio Cuniberti^{1,3}

¹Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, 01062 Dresden, Germany

²Department of Creative IT Engineering, Pohang University of Science and Technology, Pohang 790-784, Korea

³Center for Advancing Electronics Dresden (cfaed), TU Dresden, 01062 Dresden, Germany

Corresponding author: larysa.baraban@nano.tu-dresden.de

We present optoelectronic double-gate Si nanowire field-effect transistors (FETs) covered by metal ion-doped thin film. The Si nanowire FETs are fabricated by conventional top-down CMOS process designed with honeycomb structure having better gate controllability [1,2]. The channel conduction of the devices is modulated by an optically sensitive gate formed with a sol-gel derived silicate matrix including Cu^{2+} and Ni^{2+} ions (Fig.1). The film-coated devices show dramatically reduced subthreshold slope compared to conventional back-gate devices due to the polarization of ions in the film. Also, we have investigated the transfer and transconductance characteristics upon light illumination that demonstrates the channel separation in the nanowire induced by gate coupling between the back gate and the optical front gate. The optical gate bias is originated from the photoreduction of metal cations in the film. Furthermore, the devices show linear photoresponse depending on the light power density and the light spectra.

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[2] K. Kim, T. Rim, C. Park, D. Kim, M. Meyyappan and J.-S. Lee, Suspended honeycomb nanowire ISFETs for improved stiction-free performance, *Nanotechnology*, 2014, **25**(34), 345501.

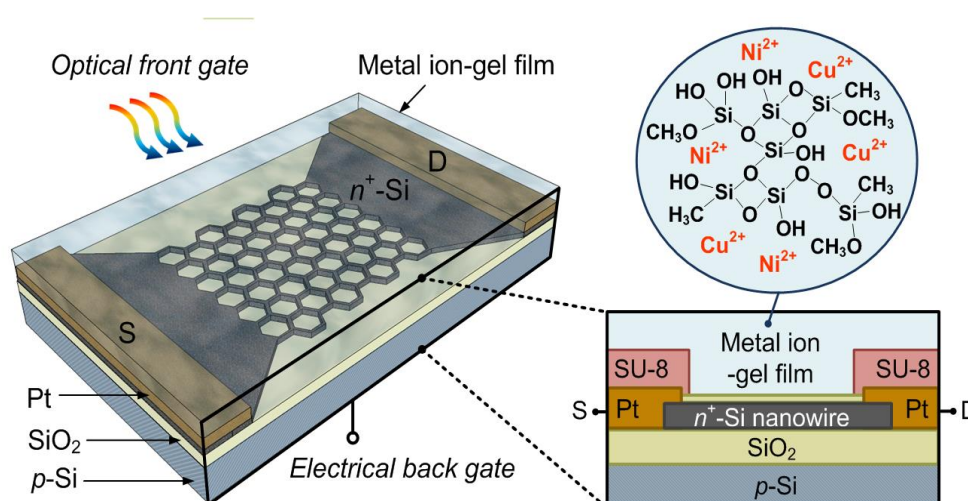


Figure 1. Schematic diagram of the metal ion-doped thin film coated Si nanowire FET

Top-down fabrication and characterization of silicon nanowire reconfigurable field effect transistors with sub 50 nm width

D. Deb^{1,3,4,6}, Y. Georgiev², M. Löffler^{3,5}, W. Weber^{3,4}, M. Helm^{1,3}, A. Erbe¹

¹Institute of Ion Beam Physics and Materials Research, HZDR, Dresden, Germany

²Tyndall National Institute, Cork, Ireland

³Centre for Advancing Electronics Dresden (cfaed), Dresden Germany

⁴Nanoelectronic materials laboratory gGmbH (NaMLab), Dresden, Germany

⁵Dresden Center for Nanoanalysis (DCNA), Dresden, Germany

⁶International Helmholtz Research School NANONET

Corresponding author: d.deb@hzdr.de

The following work illustrates top-down fabrication and characterization of reconfigurable, undoped silicon nanowire field effect transistors with Schottky junctions on silicon on insulator (SOI) substrate. The fabrication scheme is based on electron beam lithography (EBL) on a SOI substrate followed by reactive ion etching (RIE) with HSQ etch mask. In best case we fabricated nanowires with 20 nm width and 60 nm pitch.

Nickel-silicide Schottky junctions were created inside the nanowire by ni-sputtering followed by forming gas annealing. Diffusion of nickel in silicon nanowire is precisely controlled by optimizing the time of annealing. Detailed morphological analyses of the nanowires were done by transmission electron microscopy (TEM) at Dresden Center for Nanoanalysis to identify the strained deformation in silicon crystal structure due to silicidation.

Synthesis and Characterization of Polymer Functionalized Magnetic Nanoparticles for Non-destructive Testing

Mimi Hetti^{1,3,4}, Qiang Wei^{1,3}, Matthias Bartusch², Volker Neu⁵, Doris Pospiech¹, and Brigitte Voit^{*,1,3}

¹Leibniz-Institut für Polymerforschung Dresden e.V., Dresden, Germany

²Institute of Textile of Machinery and High Performance Material Technology, Faculty of Mechanical Engineering, TU Dresden, Dresden, Germany

³Organic Chemistry of Polymers, TU Dresden, Dresden, Germany

⁴International Helmholtz Research School for Nanoelectronic Networks, Dresden, Germany

⁵Leibniz Institute for Solid State and Materials Research (IFW) Dresden, Dresden, Germany

Email address: hetti@ipfdd.de

Magnetic nanoparticles were synthesized and surface grafted with poly(glycidyl methacrylate) (PGMA) for non-destructive health monitoring application. Firstly, magnetite nanoparticles (Fe_3O_4 NPs) were synthesized by precipitating ferrous and ferric chlorides with ammonium solution.¹ Fe_3O_4 NPs were then surfaced functionalized with (3-mercaptopropyl)triethoxysilane (MCTES) to form MCTES modified magnetite nanoparticles (Fe_3O_4 -MCTES NP). The resultant Fe_3O_4 -MCTES NPs were further surface grafted with PGMA² which were pre-synthesized by atom transferred radical polymerization (ATRP). The resultant Fe_3O_4 -gt-PGMA NPs form a very stable dispersion in chloroform with 124 – 178 nm of Z_{ave} . Cluster of Fe_3O_4 NPs covered with a thick but loose polymer layer is observed under TEM. Vibrating sample magnetometry reveals that the saturation magnetization (M_s) of Fe_3O_4 NPs is 77 emu/g. Upon grafted with PGMA, a high M_s value of 63 – 70 emu/g of the material can be maintained because of the high magnetite content. In addition, both the bare and modified NPs exhibit superparamagnetism. The Fe_3O_4 -gt-PGMA NPs have been blended into epoxy to form magnetic nanocomposites and can be evenly distributed in the matrix. The magnetic responsive property of the resulting materials should allow cracks or defects detection by an electromagnetic technique as non-destructive testing method.

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Multifunctional and dual-responsive polymersomes as smart nanocontainers for biomedical applications

Banu Iyisan^{1,2,3}, Dietmar Appelhans¹, Andreas Janke¹, Brigitte Voit^{1,2,3}

¹Leibniz Institut für Polymerforschung Dresden e.V., Dresden, Germany

²Organische Chemie der Polymere, Technische Universität Dresden, Dresden, Germany

³International Helmholtz Research School for Nanoelectronic Networks, Dresden, Germany

Corresponding author: iyisan@ipfdd.de

The demand for multifunctional nanovesicles is increasing greatly because of their high potential in various application fields such as drug delivery, synthetic biology and microsystem devices. The key aspect to enhance the efficiency in these areas is to fabricate robust vesicles that possess both selective recognition and responsive nature. To achieve this aim, herein multifunctional, pH-responsive and photo-crosslinked polymersomes decorated with adamantane and azide groups have been established by mixed self-assembly of suitably end-modified block copolymers. The azide functionalities are utilized in click chemistry for conjugation of nitroveratryloxycarbonyl (NVOC) protected amine molecules as photoactive moieties to provide light responsive ability. Subsequently, non-covalent immobilization of polymersomes onto convenient substrates was carried out through strong adamantane- β -cyclodextrin host-guest interaction processes. The surface-immobilized vesicles were characterized by in-situ AFM at different pH conditions to investigate the successful attachment as well as pH responsiveness. Afterwards, fs-laser illumination of the immobilized polymersomes resulted with the cleavage of NVOC moieties which led to freely accessible amine moieties on the outer shell of the vesicles. This localized photochemical reaction triggered by two-photon absorption mechanism was assessed through conjugation of a fluorescent dye to the liberated amine groups. Overall, dual responsive ability combined with the multiple functional groups make these smart polymersomes promising nanocontainers for many applications.

Electronic Transport through Au-contacted, Thiol terminated PEEB

Jeffrey Kelling¹, Torsten Sendler¹, Artur Erbe¹, Sibylle Gemming^{1,2}

¹Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

²Institute of Physics, TU Chemnitz, Chemnitz, Germany

Corresponding author: j.kelling@hzdr.de

Transport through the organic molecule 1,4-bis(phenylethynyl)-2,5-bis(ethoxy)benzene (PEEB) with thiol (SH) terminal groups, contacted by Gold electrodes, has been investigated using density functional theory (DFT) and the non-equilibrium Green's function (NEGF) method. The results confirm the existence of a single-atom contact configuration with unusually high conductance for organic molecules of $>0.1G_0$.

Electron transport in Diarylethene Switches: A combined theoretical and experimental approach

Lokamani¹, Torsten Sendler¹,
Peter Zahn¹, Sybille Gemming¹, and Artur Erbe¹

¹Institute of Ion Beam Physics and Materials Research, Dept. Scaling Phenomena
Helmholtz-Zentrum Dresden-Rossendorf e.V., Dresden

Corresponding author: m.lokamani@hzdr.de

Diarylethene, a class of photosensitive molecules which exhibit photochromism, can be switched between open- and closed-ring isomers. The open-ring isomer is non-planar with the pi-system localized on two aryl group. On the other hand, the closed-ring isomer is highly planar with the pi-conjugated-system extending over the whole molecule.

In break junction experiments diarylethene and derivatives in open and closed-ring isomer can be distinguished by a low or high conductance state with a difference in current levels of about an order of magnitude. Moreover, these molecules exhibit stable and reliable electrical characteristics in both the conductance states.

Here, we study the electronic transport properties of such derivatives at the level of single molecules. In particular, we analyze the effect of strongly electrophilic groups on conductance properties of single molecules attached to gold electrodes. A comparison to break junction experimental results is also presented.

Surface Patterning and Positioning of DNA Origami on the Nanoscale

Jonas F. Nawroth¹, Stefan Diez^{2,3}, Artur Erbe⁴, Rainer Jordan¹

¹ Professur für Makromolekulare Chemie, Department Chemie, Technische Universität Dresden, Dresden, Germany

² B CUBE – Center for Molecular Bioengineering, Technische Universität Dresden, Dresden, Germany

³ Max-Planck-Institute of Molecular Cell Biology and Genetics, Dresden, Germany

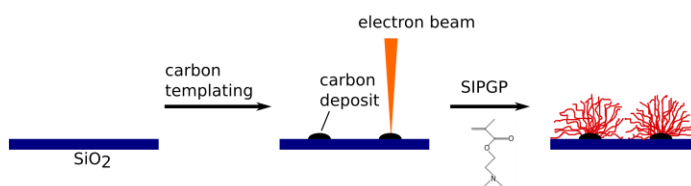
⁴ Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

Corresponding author: jonas.nawroth@tu-dresden.de

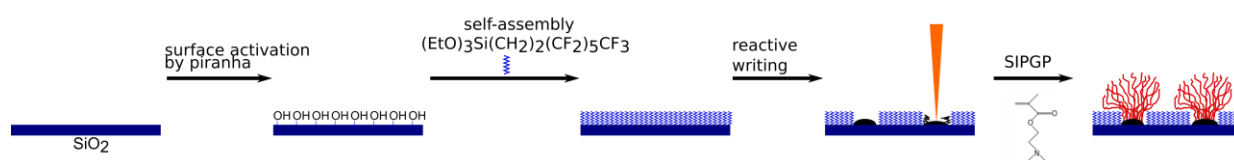
To specifically adsorb DNA origami on solid surfaces we used a combination of top-down electron beam lithography and bottom-up surface initiated polymerization. We were able to create polymer features in the sub-100 nm range, which is complementary to the dimensions of the DNA origami. The polymer patterns are formed by weakly cationic poly(N,N-dimethylaminoethyl methacrylate) brushes, which can switch from a hydrophobic to hydrophilic state under pH or temperature changes. This ability shall be used to fine-tune the binding affinity to negatively charged, hydrophilic DNA origami structure that eventually could result in improved positioning accuracy.

First results indicate higher affinity of DNA origami towards the polymer brushes compared to the hydrophobized background.

a) carbon templating (CT)



b) reactive writing (RW)



Patterning process for a) carbon templating (CT) and b) reactive writing (RW). ^[1]

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¹ J. F. Nawroth, C. Neisser, A. Erbe, R. Jordan, *in preparation*

Oligothiophenes as a promising platform for single-molecule nanoelectronics

Gözde Öktem^{1,2,3}, Anton Kiriya^{1,3}, Rainer Jordan^{2,3}

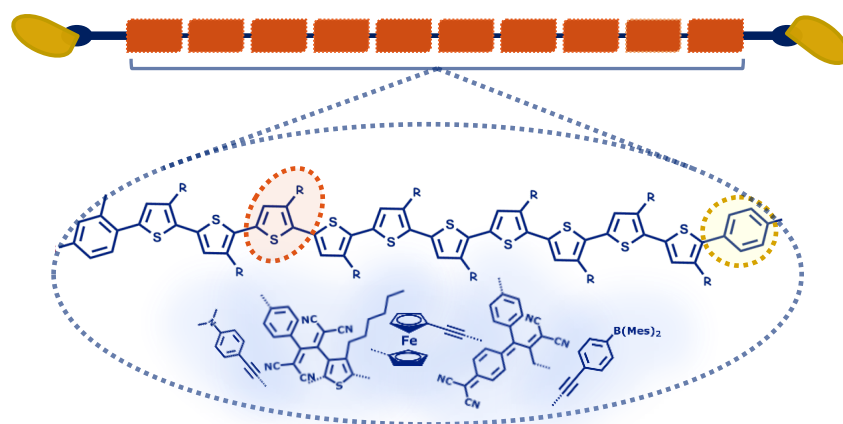
¹Leibniz-Institut für Polymerforschung Dresden e.V., Dresden, Germany

²Professur für Makromolekulare Chemie, Technische Universität Dresden, Germany

³International Helmholtz Research School for Nanoelectronic Networks, Dresden, Germany

Corresponding author: oektem@ipfdd.de

Kumada Catalyst-Transfer Polycondensation (KCTP) which involves a controlled chain-growth mechanism is utilized in the synthesis of semiconducting oligothiophenes in different conjugation lengths (from 12-mer to 28-mer) with considerably narrow dispersities (σ from 1.08-1.12), high regioregularities and well-defined bis-thiolate structures as anchoring groups without the disruption of conjugation and, therefore, with controllable and reproducible optoelectronic properties. Thio-functionalization of oligothiophenes and the gold-thiolate attachment after grafting onto gold substrate are verified by several characterization methods.



The schematic representation of oligothiophenes through break junctions and the sites that modifications studied (dotted circles)

Additionally, constructing donor-acceptor chromophores along the chain¹ and the side chains of semiconducting backbone via KCTP and several post-polymerization functionalization methods² is outlined in this study. Owing to the incorporation of the appropriate selection of electron rich and electron deficient moieties into oligo-3-hexylthiophene backbone as well as the oligomers' side chain (Figure), the optimization of oligomers' HOMO-LUMO energy levels is aimed. To link chemical design to function, semiconducting post-functionalized single oligomers will be utilized in the construction of electron-transport junctions and their possible orientations on different surfaces are further investigated.

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² Y. Li, G. Vamvounis, J. Yu, and S. Holdcroft, *Macromolecules*, **2001**, *34*, 3130.

Arrangement and characterization of functional DNA origami nanostructures for nanoelectronics

Bezu Teschome^{*,a,b}, Stefan Facsko^a, Jochen Kerbusch^a, René Hübner^a,
Kurt V. Gothelf^c and Adrian Keller^d

^aInstitute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany.

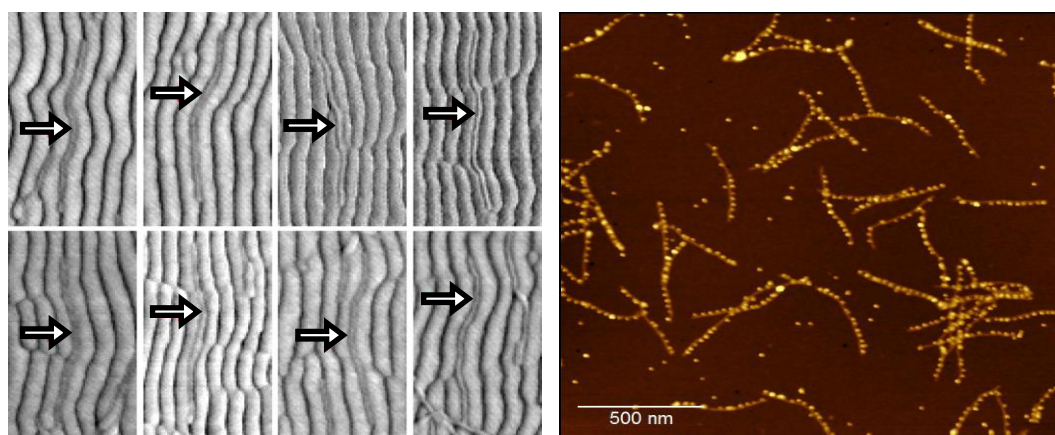
^bTechnische Universität Dresden, Mommsenstraße 13, 01069 Dresden, Germany.

^cDanish National Research Foundation: Centre for DNA Nanotechnology (CDNA) at Interdisciplinary Nanoscience Center (iNANO) and Department of Chemistry, Aarhus University, 8000 Aarhus C, Denmark.

^dTechnical and Macromolecular Chemistry, University of Paderborn, Warburger Str. 100, 33098 Paderborn, Germany.

Corresponding author: b.teschome@hzdr.de

DNA origami has become a key technique for designing well-defined nanostructures with any desired shape and for the controlled arrangement of functional nanostructures with few nanometer resolution. These unique features make DNA origami nanostructures promising candidates for use as scaffolds in nanoelectronics and nanophotonics device fabrication. This talk will highlight some of results from our work on the arrangement and characterization of functional DNA origami nanostructures for nanoelectronics. First, a new compelling approach to generate ordered arrays of DNA origami nanotubes on topographically patterned Si surfaces will be introduced¹. Then, the high-yield synthesis of high-density gold nanoparticle (AuNP) arrangements on DNA origami nanotubes with few unbound background nanoparticles will be presented. The high yield of AuNP assembly was achieved by careful control of the buffer concentration and the hybridization time on Si surface. Finally, also the assembly of heterogeneous nanostructures, i.e. 5 nm gold nanoparticles (AuNPs) and 10 nm semiconductor quantum dots (QDs), on a single DNA origami will be demonstrated.



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Your Notes

Poster abstracts

Yuriy Aleksandov

Electrical detection of the ferromagnetic resonance in an individual, nanoscale magnetic stripe (see talks)

Himani Arora

Amorphous indium-gallium-zinc-oxide as electron transport layer in organic photodetectors

Wajid Awan

Electrical Transport properties of two dimensional CVD Molybdenum disulphide (MoS_2)

Eunhye Baek

Optoelectronic Double-Gate Modulation in Metal Ion-doped Thin Film-coated Si Nanowire FETs (see talks)

Dipjyoti Deb

Top-down fabrication and characterization of silicon nanowire reconfigurable field effect transistors with sub 50 nm width (see talks)

Florian Fuchs

Electronic Structure and Transport Properties of Thin Silicon Nanowires

Florian Günther

Contribution of the stacking interaction to the planarity of polymers

Mimi Hetti

Synthesis and Characterization of Polymer Functionalized Magnetic Nanoparticles for Non-destructive Testing (see talks)

Banu Iyisan

Multifunctional and dual-responsive polymersomes as smart nanocontainers for biomedical applications (see talks)

Jeffrey Kelling

Electronic Transport through Au-contacted PEEB

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Memristive phenomena in multiferroic materials

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Surface Patterning and Positioning of DNA Origami on the Nanoscale

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DFT Simulation of STM image of aromatics monomers on metallic surfaces

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Oligothiophenes as a promising platform for single-molecule nanoelectronics (see talks)

Perumallapelli Goutham Raj

Orthogonal Solvent Engineering Treatment of Perovskite thin film for Improved Morphology, Efficiency and Stability in Planar Heterojunction Perovskite Solar Cells

Julian Schütt

Real-Time impedance sensing of microorganisms using gold nanowires

Torsten Sandler

Induced Conductance in Single-Molecule Junctions

Wenbo Sheng

Conductive polymer carpets as sensors

Dmitry Skidin

Cyclic organosulfur molecules as precursors for 2D surface complexes

Bezu Teschome

Arrangement and characterization of functional DNA origami nanostructures for nanoelectronics (see talks)

Panpan Zhang

Synthesis and modification of MoS₂ monolayers for photoswitches

Amorphous indium-gallium-zinc-oxide as electron transport layer in organic photodetectors

H. Arora,^{1,2} P. E. Malinowski,¹ A. Chasin,¹ D. Cheyns,¹ S. Steudel,¹ S. Schols,¹ and P. Heremans^{1,3}

¹IMEC, Kapeldreef 75, 3001 Leuven, Belgium

²Phelma-Grenoble INP, 3 Parvis Louis Neel, 38016 Grenoble Cedex 01, France

³ESAT, Katholieke Universiteit Leuven, Kasteelpark Arenberg 10, B-3001 Leuven, Belgium

Corresponding author: himani.arora.06@gmail.com

Amorphous indium-gallium-zinc-oxide (a-IGZO) is demonstrated as an electron transport layer (ETL) in a high-performance organic photodetector (OPD). Dark current in the range of 10 nA/cm² at a bias voltage of -2V and a high photoresponse in the visible spectrum were obtained in inverted OPDs with poly(3-hexylthiophene) and phenyl-C₆₁-butyric acid methyl ester active layer. The best results were obtained for the optimum a-IGZO thickness of 7.5 nm with specific detectivity of 3x10¹² Jones at the wavelength of 550 nm. The performance of the best OPD devices using a-IGZO was shown to be comparable to state-of-the-art devices based on TiO_x as ETL, with higher rectification achieved in reverse bias. Yield and reproducibility were also enhanced with a-IGZO, facilitating fabrication of large area OPDs. Furthermore, easier integration with IGZO-based readout backplanes can be envisioned, where the channel material can be used as photodiode buffer layer after additional treatment.

Stacking different 2D materials to fabricate a high mobility transistor

(PhD topic at HZDR)

In recent years, several 2D semiconducting materials like MoS₂, WSe₂, silicene, germanene, phosphorene etc. have been produced and intensively studied. Their semiconducting properties allow the development of two-dimensional structures, whose electronic properties can be tuned. By fabricating gate electrodes on the 2D materials, field effect transistors have been demonstrated. However, so far the transistors based on these materials suffered some serious drawbacks.

In the field of 2D materials, one of the most exciting frontiers is stacking them together which have opened up new opportunities. Different 2D materials are combined in such a way that all their different advantages can be properly utilized to achieve desired application. Successful fabrication of solar cells and photodetectors from the stacking of graphene and MoS₂ is one example. In this PhD study, the focus is to sandwich different 2D layers to fabricate a high mobility transistor. One of major part will comprise of selecting various 2D materials, whose different properties can complement each other for fabricating a successful stack. An attempt will also be made to dope these 2D layers (by using ion planation etc.) to enhance their properties which could be beneficial for the final device.

Title: Electrical Transport properties of two dimensional CVD Molybdenum disulphide (MoS_2)

Wajid A. Awan

Two dimensional materials are attractive for the use in next-generation nanoelectronic devices as compared to one dimensional material because it is relatively easy to fabricate complex structures from them. After the successful discovery of graphene, recently the layered 2D semiconducting Transition metal dichalcogenides come into the picture and got a place in a wide range of novel applications as well as in basic research. Strikingly, MoS_2 receives significant attention since it undergoes transition from indirect bandgap (bulk form) to a direct bandgap (1.2eV) semiconductor if thinned out to a single atomic layer. The bandgap is an essential property for the tunable 2-D nanodevices. We performed the electrical transport measurements at room temperature for the CVD grown MoS_2 on SiO_2/Si substrate. The standard Electron beam lithography (EBL) process was used to pattern the Gold (Au) metal contacts on MoS_2 flakes. For the purpose of sample characterization, we performed the Atomic Force Microscopy (AFM) and Raman Spectroscopy techniques respectively which confirm the single layer thickness of CVD MoS_2 triangular flakes on SiO_2/Si substrate. Future work will be based on the low temperature dependence measurements and magneto transport measurements. Further experiments will be the modification of the 2-dimensional layer by controlled ion irradiation introducing the single defects into the semiconducting layers and by putting such structures on thin SiO_2 layers with conducting silicon underneath for the application of gate voltage. The future motivation is to explore under what conditions modifications can be introduced by doping process in such 2- dimensional materials.

Electronic Structure and Transport Properties of Thin Silicon Nanowires

Florian Fuchs^{1,2,3}, Sibylle Gemming^{1,3}, Jörg Schuster⁴

¹Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

²Center for Advancing Electronics Dresden, Dresden, Germany

³Faculty of Natural Science, Technische Universität Chemnitz, Chemnitz, Germany

⁴Fraunhofer Institute for Electronic Nano Systems, Chemnitz, Germany

Corresponding author: f.fuchs@hzdr.de

Silicon nanowires (SiNWs) are promising candidates as building blocks for electronic devices. They allow for a further miniaturization because silicon is already well established in technology and some existing technologies can be reused.

For the simulation of SiNWs, numerical device simulations, based on the silicon bulk band structure, are often used. When the diameter is reduced, however, atomistic quantum simulations become mandatory at some point.

In the present work, thin hydrogen-passivated SiNWs with diameters between 1 and 6 nm are studied by means of density functional theory. It is shown that the band gap approaches the bulk value in the limit of infinitely thick nanowires and increases for thin wires due to quantum confinement. Using a radially resolved density of states it is demonstrated, that the density of states is highest in the nanowire center, where most of the current transport would occur, and decreases near the surface. Comparing the density of states between SiNWs with different diameters, the transition to bulk silicon can be observed (see figure). This justifies the use of bulk band structure approximations for thicker SiNWs, but also highlights the need for atomistic quantum simulations in case of thin ones.

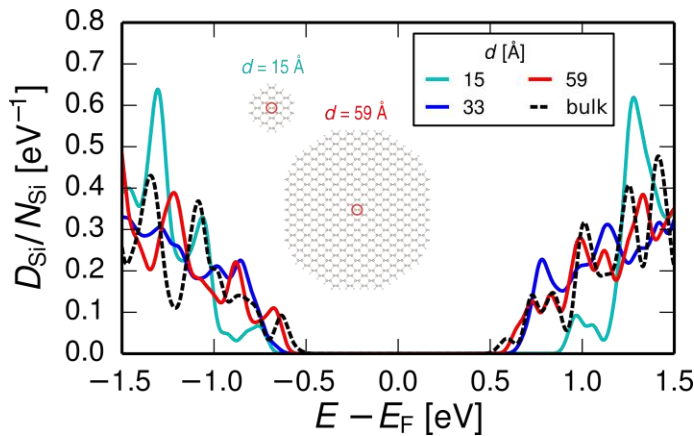


Figure: Density of states per silicon atom $D_{\text{Si}}/N_{\text{Si}}$ in the middle of SiNWs with different diameter d (the considered atoms are circled). The black dashed line corresponds to the bulk limit of silicon.

Contribution of the stacking interaction to the planarity of polymers

Florian Günther^{1,2}, Anton Kiriya^{2,3}, Sibylle Gemming^{1,4}, Gotthard Seifert²

¹ Institute of Ion Beam Physics and Materials Research, HZDR, Dresden, Germany

² Faculty of Science, Theoretical Chemistry, TU Dresden, Dresden, Germany

³ Leibniz Institute of Polymer Research Dresden (IPF), Dresden, Germany

⁴ Faculty of Natural Sciences, Institute of Physics, TU Chemnitz, Chemnitz Germany

Corresponding author: f.guenther@hzdr.de

A high degree of molecular planarity is of crucial importance to design organic polymers with enhanced semiconducting properties. Commonly, the delocalized π -system is considered as the driving force for the planarity of conjugated polymers. In this study, however, an alternative approach is discussed: In a crystal phase, the conformational freedom is much lower than in amorphous systems. Thus, the contribution of the stacking interaction to the planarity of polymers is under investigation. Based on density functional theory calculations, the energy for distorting the planarity of thiophene and thienothiophene based dimers, oligomers, and polymers are evaluated. For this, the behavior of amorphous structures is modeled by calculating single isolated systems. The crystal phase, however, is studied considering periodically stacked molecules.

Electronic Transport through Au-contacted PEEB

Jeffrey Kelling¹, Torsten Sessler¹, Artur Erbe¹, Sibylle Gemming^{1,2}

¹Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

²Institute of Physics, TU Chemnitz, Chemnitz, Germany

Corresponding author: j.kelling@hzdr.de

Transport through the organic molecule 1,4-bis(phenylethynyl)-2,5-bis(ethoxy)benzene (PEEB) has been investigated using Density functional Theory (DFT) and the Non-Equilibrium Green's Function (NEGF) approach in order to explain results of experiments employing the mechanically controlled break junction (MCBJ) technique. The molecule was studied with various terminal groups (NH₂, SH and CN) which lead to different conductance values when attached to Gold electrodes. The effect of different contact geometries was studied in simulations, allowing predictions on the most likely contact geometries occurring in experiments.

Memristive phenomena in multiferroic materials

Lokamani Lokamani¹, Peter Zahn¹, Nicola Spaldin², and Sybille Gemming¹
¹Institute of Ion Beam Physics and Materials Research, Dept. Scaling phenomena,
Helmholtz-Zentrum Dresden-Rossendorf e.V., Dresden
²Dept. Materials Theory, ETH Zürich

Corresponding author: m.lokamani@hzdr.de

The project aims at quantifying the conductivity change along domain walls in multiferroic SrMnO₃ and YMnO₃ based films induced by oxygen vacancies with the help of first-principles modeling.

We present here preliminary work on the electronic structure of SrMnO₃ and YMnO₃ using ab-initio methods. Additionally, the effect of induced oxygen vacancies on the associated structural-, electronic- and magnetic-change in bulk properties is presented. In addition, we present preliminary work on domain and grain boundary models, polar domain boundary models (90° and 180°) in these materials.

Surface Patterning and Positioning of DNA Origami on the Nanoscale

Jonas F. Nawroth¹, Stefan Diez^{2,3}, Artur Erbe⁴, Rainer Jordan¹

¹ Professur für Makromolekulare Chemie, Department Chemie, Technische Universität Dresden, Dresden, Germany

² B CUBE – Center for Molecular Bioengineering, Technische Universität Dresden, Dresden, Germany

³ Max-Planck-Institute of Molecular Cell Biology and Genetics, Dresden, Germany

⁴ Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

Corresponding author: Jonas.nawroth@tu-dresden.de

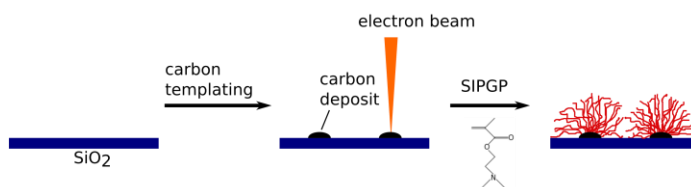
In the Biomolecular-assembled circuits path, within the excellence cluster “Center for Advancing Electronics Dresden” (cfaed), our goal is to combine top-down with bottom-up strategies to achieve even smaller structures. The circuits will be designed by metalized DNA origamis, but the challenge for this very project is to pattern the Si-based substrate in a way that the DNA will attach specifically and possible reversibly.

The top-down method of choice is electron beam lithography (EBL). With this technique it is possible to write structures with a resolution down to 5 nm. The generated structures are carbon deposits that can be used for further functionalization.

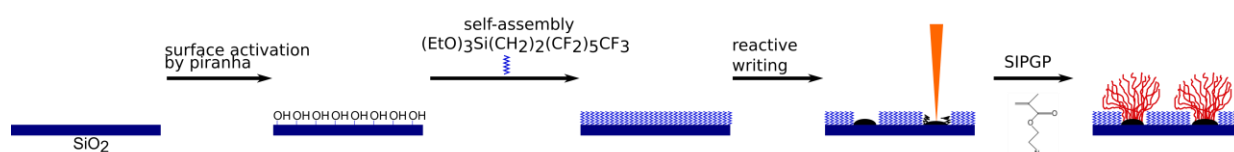
Functionalization will be achieved by self-initiated photografting and photopolymerization (SIPGP). This radical polymerization uses the proton abstraction from the surface that occurs under UV-irradiation with excited vinyl monomers. This generates surface bound radicals that lead to polymer brushes growing from the surface. However, this does not work on surfaces where the bonding dissociation energy is too high (e.g. SiOH or perfluorinated silanes), but it does on the carbon deposit.

With this difference in functionality it will be possible to precisely tune, not only the position of the DNA on the substrate but also, depending on the used monomer, the binding affinity to the brush.

a) carbon templating (CT)



b) reactive writing (RW)



Patterning process for a) carbon templating (CT) and b) reactive writing (RW). ^[1]

References

¹ J. F. Nawroth, C. Neisser, A. Erbe, R. Jordan, *in preparation*

DFT Simulation of STM image of aromatics monomers on metallic surfaces

Seddigheh Nikipar

Institute for Materials Science and Max Bergmann Center of Biomaterials,
Dresden, Germany
Faculty of Mechanical Science and Engineering, TU Dresden, Dresden, Germany

Corresponding author: snikipar@nano.tu-dresden.de

Advances in the experimental techniques have enabled researchers to manipulate atomic sized materials. One promising approach is surface assisted synthesis in UHV condition which provides effective method to access wide range of Nano-scale materials in controllable way. The on-surface polymerization process allows for the engineering of manifold extended 2D materials, especially the prospect to fabricate molecular wires and Graphene nanoribbons in different widths.

Therefore, the on-surface synthesis of 1D and 2D polymers has attracted considerable attention over the recent years. In general, scanning tunneling microscopy (STM) has been the main tool for exploring surface-confined polymerization. In order to support the experiments and to predict further technological advance, theoretical modeling of these structure is demanded. In this way sophisticated ab initio computational methods have been developed to explore these novel structures.

In the present work we employed state-of-the-art atomistic simulations based on density functional theory (DFT) and Tersoff-Hamann approach which is based on the quantum mechanical effect of electron tunneling to simulate STM topographs, dI/dV spectroscopy, electron density of states in chrysene derivative monomer on Au(111) surface. The outcome shows good agreement with experimental results.

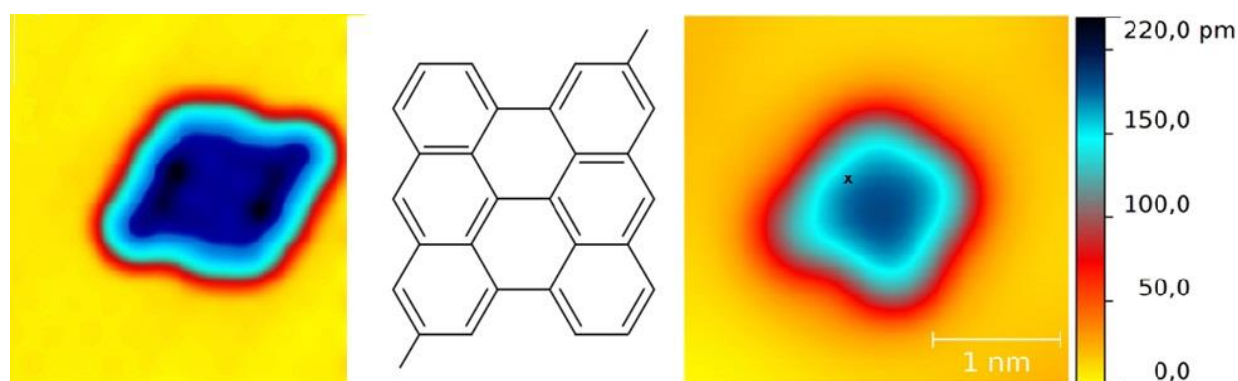


Figure : Chrysene derivative on Au(111) after heating to 170 °C; Image sizes: 3nm x 3nm; Bias: 0.5 V; Current: 100 pA; Left: theoretical calculation; Right: experimental result;

Orthogonal Solvent Engineering Treatment of Perovskite thin film for Improved Morphology, Efficiency and Stability in Planar Heterojunction Perovskite Solar Cells

P. Goutham Raj and Jin Jang*

Advance Display Research Center, Department of Information Display, Kyung Hee University, Dongdaemun-gu, Seoul, Korea.

*Corresponding author: jang@khu.ac.kr

Orthogonal solvent engineering technique for planar heterojunction perovskite solar cells is an efficient way to achieve uniformly controlled grain morphology for perovskite films. Planar heterojunction perovskite ($\text{CH}_3\text{NH}_3\text{PbI}_3$) solar cells have been fabricated using orthogonal solvent engineering treatment. Here solvent “A” has been used as an orthogonal solvent for treatment. Solvent A is chosen by checking whether it dissolves perovskite precursor materials and its miscibility in perovskite solvents (DMSO: GBL). Orthogonal solvent removes excess solvent from the perovskite, which encourages super saturation leading to fast nucleation. On further thermal annealing or curing, the uniform crystalline perovskite is formed. Solar cells with solvent treatment exhibited higher power conversion efficiency (PCE) of 9.06% when compared to untreated which yielded PCE of 6.10%. This increase in efficiency is due to improved film morphology of perovskite layer after solvent treatment which has been revealed under UV-Vis spectroscopy, SEM images, X-ray diffraction and impedance spectroscopy. Light and dark J-V characteristics are shown in figure 1. Moreover, the devices with solvent treatment exhibited stability over 100 days

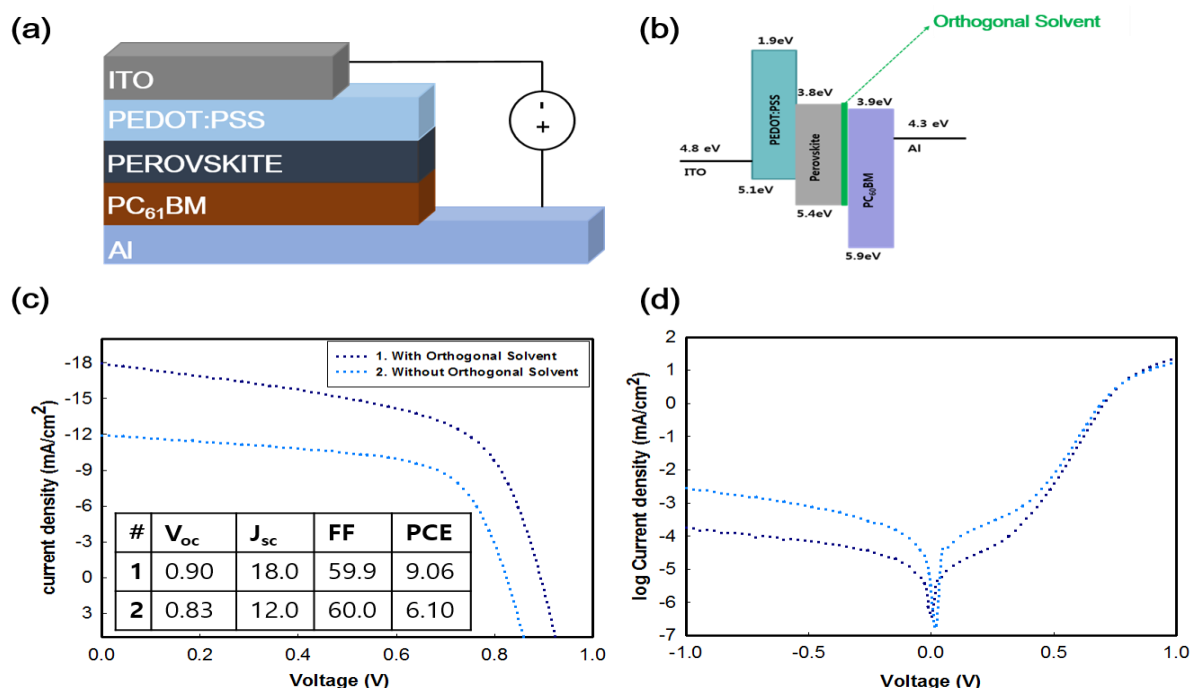


Figure 1. (a) Schematic diagram of the fabricated perovskite solar cells, (b) energy band diagram of the entire device, (c) and (d) are light and dark J-V characteristics of the fabricated perovskite solar cells measured under illumination of AM1.5 stimulated solar radiation.

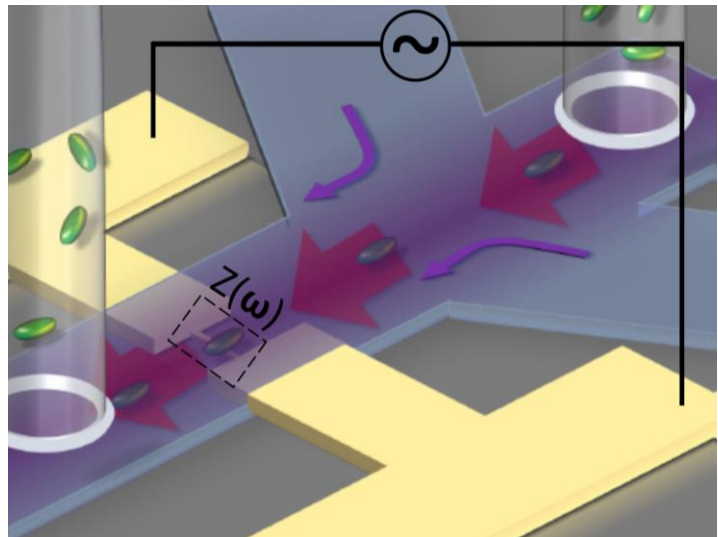
Real-Time impedance sensing of microorganisms using gold nanowires

Julian Schütt¹, Larysa Baraban¹, Gianaurelio Cuniberti¹

¹Institute for Materials Science and Max Bergmann Center of Biomaterials,
Dresden University of Technology, Budapester Str. 27, 01062 Dresden, Germany

Corresponding author: julian.schuett@nano.tu-dresden.de

Detection of pathogens at low concentrations and sample volumes is one of the mainstreams in the current biomedical research due to the distinct demographic changes and wide spreading of the chronic and severe illnesses. Conventional pathogen detection approaches like flow cytometry, qPCR and microarrays require high sample volumes, trained personnel, long detection times and their usage is furthermore limited to suitable facilities. However, there is a high demand for precise, cheap and portable sensor devices for application in the environment where the patient needs a proper treatment without available qualified personnel and hospitals, e.g. in developing countries. To overcome the limitations of common techniques, we faced the challenge to establish a MEMS-sensor capable of single cell detection using a dynamic gold nanowire-based impedance analysis (See figure). The detection of cells is realized in flow, employing the cytometry principle. The use of nanowires allows higher sensitivity and selectivity due to electric field enhancement at the nanowire tips as well as higher signal-to-noise ratio by ballistic electron transport at the sensing nanostructures¹. Next to its capability of pathogen detection, this technique is able to contribute to real-time cancer phenotyping² and label-free DNA quantification³ at low volumes. Here, we present first results in fabrication and sensing experiments. The gold nanowires are fabricated top-down using electron-beam lithography (EBL) and integrated into the macro-electrode design via lift-off based optical lithography. The transport system consists of a 3D focusing microfluidic structure, which focuses the analyte solution between the nanowires. We demonstrate the detection events of single cells at the proof of concept level.



Schematic illustration of the sensing device. The analyte solution is guided between the gold nanowire electrode pair thereby altering the impedance of the sensing structure.

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Induced Conductance in Single-Molecule Junctions

Torsten Sendler¹, Katharina Luka-Guth², Matthias Wieser¹, Lokamani¹, Jannic Wolf³, Michael Mortensen⁴, Kurt Gothelf⁴, Manfred Helm¹, Sibylle Gemming¹, Jochen Kerbusch¹, Elke Scheer², Thomas Huhn³, Artur Erbe¹

¹Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

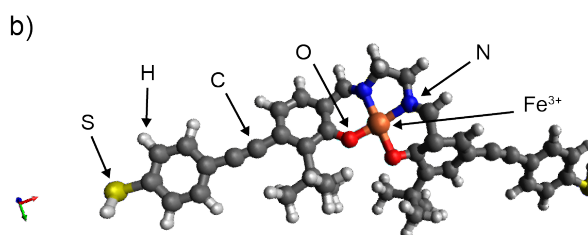
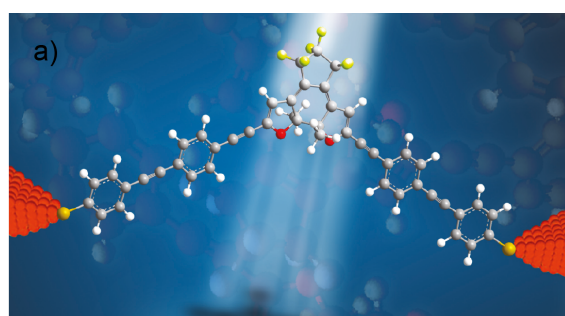
²Department of Physics, Universität Konstanz, Germany

³Department of Chemistry, Universität Konstanz, Germany

⁴Centre for DNA Nanotechnology, Department of Chemistry and Interdisciplinary Nanoscience Center, iNANO, Aarhus, Denmark

Corresponding author: t.sendler@hzdr.de

The goal of molecular electronics is the realization of integrated molecular circuits. For this purpose reliable contacts to single molecules have to be built and the characteristics of those junctions need to be investigated. We have demonstrated that the mechanically controllable break junction (MCBJ) technique is a suitable tool to study the electrical transport through molecular junctions and to analyze the electronic structure of the molecules.^[1] Furthermore, based on the use of complex molecules, we are able to control the conductance of single molecular junctions. On the one hand, molecular switches (a) are transformed *in-situ* from a non-conductive “off”- to a conductive “on”-state via light-irradiation of a well-defined wavelength.^[2] On the other hand molecule-metal complexes (b) are turned from an isolating to a conductive state by introducing metal centers into the molecular structures. The findings provide a significant contribution to the development of functional molecular junctions.



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Conductive polymer carpets as sensors

Wenbo Sheng, Rainer Jordan*

Professur für Makromolekulare Chemie, Department Chemie, Technische Universität Dresden,
MommSENstrasse 4, 01062 Dresden, Germany

Corresponding author: rainer.jordan@tu-dresden.de

Graphene is a true 2-dimensional material with exceptional structural, chemical, and electrical properties which make it a highly promising candidate for biosensing and bioelectronics.^[1] Polymer brushes can improve transport properties and provide clear pathways for charge transport in the direction normal to the substrate.^[2] In order to utilize the full potential of graphene and polymer brushes, our group has achieved to graft the polymer brushes on graphene.^[3] Then we have used a simple method to graft the conductive polymer brushes on graphene via a combination of self-initiating photografting and photopolymerization (SIPGP) and surface-initiated Kumada catalyst transfer polycondensation (SI-KCTP). Inspired by graphene and conductive polymer brushes with improved sensitivity towards external stimuli,^[4] this project will prepare graphene-based conductive polymer carpets (It can be transferred to any substrates due to the flexible of graphene, so called “conductive polymer carpet”, as shown in Figure 1.) with different functional groups as ultrasensitive chemical sensors. The sensors will be used for the detection of volatiles as well as biomolecules in liquids. It is expected that they will find practical applications in the electrochemical and biomedical fields.^[5]

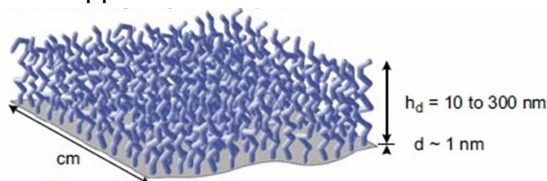


Figure 1. Polymer carpets.^[6]

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Cyclic organosulfur molecules as precursors for 2D surface complexes

Dmitry Skidin¹, Frank Eisenhut¹, Justus Krüger¹, Francesca Moresco^{1,2},
Xinliang Feng^{2,3}, and Gianaurelio Cuniberti^{1,2}

¹Institute for Materials Science, Max Bergmann Center of Biomaterials, and

²Center for Advancing Electronics Dresden, and

³Department of Chemistry and Food Chemistry, TU Dresden, 01062 Dresden, Germany

Corresponding author: dskidin@nano.tu-dresden.de

The class of organosulfur molecules presents a wide interest for the scientific community during the last decades. Owing to their strong binding properties to the gold surfaces they find many applications in the fields of surface functionalization, biological molecules immobilization and molecular electronics. Self-assembly of sulfur-containing molecules (mostly alkanethiols) on gold surfaces has been investigated quite extensively, and it has been recently shown that gold adatoms play a key role for this process [1]. However, its mechanism as well as self-assembly of organosulfur cyclic compounds is not yet fully understood.

In the present work gold adatom mediation is employed to form 2D surface meta-organic frameworks. Perbenzylthi coronene and perbenzylthiobenzene are chosen as precursors because they both have an aromatic core surrounded by 12 and 6 sulfur-containing sidegroups respectively and thus provide a good template for a coordinated network. The precursors are deposited on the Au(111) single-crystal surface and subsequently heated to induce diffusion process. All the measurements are conducted using scanning tunneling microscopy (STM) at the temperatures around 5 K and base pressure not worse than 10^{-10} mbar.

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Synthesis and modification of MoS₂ monolayers for photoswitches

Panpan Zhang, Prof. Dr. Xinliang Feng

Department of Chemistry and Food Chemistry, Faculty of Science,
Dresden University of Technology, 01062 Dresden, Germany

Corresponding author: xinliang.feng@tu-dresden.de

Graphene, as one of the most fascinating research topics with unique structures and outstanding properties, has shown enormous fundamental and technological applications. Inspired by the great success of graphene, other two-dimensional (2D) atomic crystals with mono or few layers have been paid much attention in recent years. As the typical 2D nanostructures with a large lateral size and a small thickness, molybdenum disulfide (MoS₂) nanosheets exhibit unusual properties and offer a broad view of study due to their high surface area, controlled exposed crystal facets and diverse compositions. Firstly, the efficient synthesis should be developed by using top-down exfoliation (lithium intercalation, surfactant and liquid-assisted) and bottom-up techniques (hydrothermal synthesis and vapor transportation). Then, we will design and synthesize azobenzene molecule with thiol-terminate, which is functional with photoisomerization and conjugated to MoS₂ monolayers. Finally, the exfoliated MoS₂ monolayer with ligand conjugation can not only have semi-conducting property but also possess photoresponse performance. Therefore, it can be used as electronic device such as photodetector, transistor, and photoswitch.

Your Notes

Participants

updated

25.09.2015 (PZ)

Name	First Name	Title	Institution
Aleksandrov	Yuriy	Mr.	HZDR
Arora	Himani	Ms.	HZDR
Awan	Wajid	Mr.	HZDR
Baek	Eunhye	Ms.	TUD
Baraban	Larysa	Dr.	TUD
Cuniberti	Gianaurelio	Prof. Dr.	TUD
Deb	Dipjyoti	Mr.	HZDR
Erbe	Artur	Dr.	HZDR
Fuchs	Florian	Mr.	HZDR
Gemming	Sibylle	Prof. Dr.	HZDR
Gothelf	Kurt	Prof. Dr.	Aarhus Univ
Günther	Florian	Mr.	HZDR
Helm	Manfred	Prof. Dr.	HZDR
Herrmann	Carmen	Prof. Dr.	Hamburg Univ
Hetti	Mimi	Ms.	IPF
Huhn	Thomas	Dr.	Konstanz Univ
Iyisan	Banu	Ms.	IPF
Keller	Adrian	Dr.	Paderborn Univ
Kelling	Jeffrey	Mr.	HZDR
Kiriy	Anton	Dr.	TUD
Lokamani	Mani	Mr.	HZDR
Metzger	Robert	Prof. Dr.	Alabama Univ
Meyyapan	Meyya	Prof. Dr.	NASA Ames Res Cent
Moresco	Francesca	Dr.	TUD
Nawroth	Jonas	Mr.	TUD
Nikipar	Seddigheh	Ms.	TUD
Öktem	Gözde	Ms.	IPF
Perumallapelli	Goutham Raj	Mr.	IPF
Ryndyk	Dmitriy	Dr.	TUD
Scheer	Elke	Prof. Dr.	Konstanz Univ
Schuster	Jörg	Dr.	FhG ENAS Chemnitz
Schütt	Julian	Mr.	TUD
Sendler	Torsten	Mr.	HZDR
Sheng	Wenbo	Ms.	TUD
Skidin	Dmitry	Mr.	TUD
Teschome	Bezu	Mr.	HZDR
Voit	Brigitte	Prof. Dr.	IPF
Zacharias	Helmut	Prof. Dr.	Münster Univ
Zahn	Peter	PD Dr.	HZDR
Zhang	Panpan	Mr.	TUD

hZDR



HELMHOLTZ
| ZENTRUM DRESDEN
| ROSSENDORF

