

# **IHRS NANONET ANNUAL WORKSHOP 2013**

October 10, 2013 Dresden, Germany



# International Helmholtz Research School for Nanoelectronic Networks



# **IHRS NANONET Annual Workshop 2013**

10 October 2013, Dresden, Germany















### Venue and organization

#### Venue

Helmholtz-Zentrum Dresden-Rossendorf Bautzner Landstrasse 400, 01328 Dresden, Germany

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International Helmholtz Research School for Nanoelectronic Networks (IHRS NANONET)

Helmholtz-Zentrum Dresden-Rossendorf

Bautzner Landstrasse 400, 01328 Dresden, Germany

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### Greeting

Dear Participants,

Welcome to the first workshop of the International Helmholtz Research School for Nanoelectronic Networks (IHRS NANONET). The IHRS NANONET is an interdisciplinary research school in the field of molecular electronics open to outstanding students of all nationalities with backgrounds in physics, chemistry, electrical engineering, and materials science. The 3-years PhD programme includes independent research work in a project involving different branches of science and engineering and a well-structured scientific curriculum providing for a comprehensive training in technical and professional skills.

Dresden is the ideal location for such a research school: being the largest European microand nanoelectronics cluster, more than 2,100 companies employing in total 51,000 people are
working in the city and the surrounding area along the whole value chain of information and
communication technologies. But not only in industry Dresden developed into a leading center
of modern electronics. A dense research and teaching network made up of TU Dresden and
numerous non-university research institutions from the Max Planck Society, the Leibniz
Association, the Fraunhofer Society and the Helmholtz-Zentrum Dresden-Rossendorf, are
dedicated to working on electronic technologies for tomorrow. The IHRS NANONET involves the
major Dresden players in its active, exciting and visionary area of electronics and keeps close
connections to the strong local industrial landscape in order to provide the students an optimal
environment to build a future in research in micro- and nanoelectronics.

The first student of our school joined in October 2012, exactly one year ago. Therefore, this workshop gives the ideal opportunity to review the progress which we have made during the start-up phase of our research school in the field of molecular nanoelectronics. Up to date 12 doctoral candidates coming from 7 different countries have joined the IHRS NANONET. We will present highlights of their research in 5 talks during the workshop, each of the candidates will show a poster with the progress of their projects. Additionally, we are proud and happy that renowned experts in our field are joining us presenting talks and in the discussions during the breaks and at the posters. We hope that all of you will have an inspiring time at the workshop in Dresden-Rossendorf.

Dr. Artur Erbe Speaker IHRS NANONET Helmholtz-Zentrum Dresden-Rossendorf Prof. Dr. Gianaurelio Cuniberti Deputy speaker IHRS NANONET Technische Universität Dresden

# Program

09:00 – 09:15	Welcome / Registration
	Chairman: Manfred Helm
09:15 – 09:25	Artur Erbe (Helmholtz-Zentrum Dresden-Rossendorf) International Helmholtz Research School for Nanoelectronic Networks
09:25 – 10:05	Keynote talk: <b>Robert M. Metzger</b> (University of Alabama, USA)  Inching towards four-electrode contacts to a single molecule
10:05 – 10:45	Keynote talk: <b>Herre van der Zant</b> (TU Delft, The Netherlands) Single-molecule electronic components
10:45 – 11:00	Coffee break
	Chairman: Gianaurelio Cuniberti
11:00 – 11:40	Keynote talk: <b>Heike R. Riel</b> (IBM Research Zurich, Switzerland) tbd
11:40 – 12:20	Keynote talk: <b>Kurt V. Gothelf</b> (Aarhus University, Denmark)  DNA-Programmed assembly of conjugated polymers
12:20 – 13:30	Lunch break
	Chairman: Stefan Facsko
13:30 – 13:55	Invited talk: <b>Gianaurelio Cuniberti</b> (TU Dresden)  A bottom-up route to enhance thermoelectric figures of merit in graphene nanoribbons
13:55 – 14:20	Invited talk: <b>Francesca Moresco</b> (TU Dresden)  STM controlled manipulation of single molecules and molecular structures
14:20 – 14:45	Invited talk: <b>Anton Kiriy</b> (Leibniz Institute of Polymer Research Dresden)  Controlled polycondensation at work: synthesis of well-defined semiconducting polymers for needs of organic electronics
14:45 – 15:00	Coffee break
	Chairman: Artur Erbe
15:00 – 15:25	Invited talk: <b>Adrian Keller</b> (Helmholtz-Zentrum Dresden-Rossendorf)  DNA origami-based nanodevices

15:25 – 15:50	Invited talk: <b>Jochen Grebing</b> (Helmholtz-Zentrum Dresden-Rossendorf) Electronic devices based on nanowires		
15:50 – 17:20	Poster session with coffee	Chairmen: Artur Erbe & Gianaurelio Cuniberti	
17:40 – 18:00	Poster prize ceremony		
18:00	Dinner		

# Keynote talk abstracts

**Robert M. Metzger** (University of Alabama, USA) *Inching towards four-electrode contacts to a single molecule* 

**Herre van der Zant** (TU Delft, The Netherlands) Single-molecule electronic components

**Heike R. Riel** (IBM Research Zurich, Switzerland) *tbd* 

**Kurt V. Gothelf** (Aarhus University, Denmark) DNA-Programmed assembly of conjugated polymers

### Inching towards four-electrode contacts to a single molecule

Robert M. Metzger

Laboratory for Molecular Electronics, Department of Chemistry, University of Alabama, Tuscaloosa, AL 35487-0336, USA

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This laboratory has been studying **rectification** of electrical current by Langmuir-Blodgett, Langmuir-Schaefer and self-assembled monolayers (SAMs) between Au electrodes for several decades [1], [2]. Recently we have found a new SAM rectifier, which however changes its asymmetric current peak in the current  $I - voltage\ V\ (IV)$  curves from positive to negative bias if the bias exceeds  $\pm\ 2\ V\ [3]$ ; this turn-around, with donor levels at low bias, then both donor and affinity levels getting involved at high bias, is not new [4].

We have also established the necessary theoretical conditions for a single molecule connected to three electrodes to be a **unimolecular amplifier** (UA): the IV curves can be displaced by the bias on the central "control" electrode, thanks to bipolar junction effects and to field effects [6].

This study has inspired an experimental test of UA; the first (ongoing) mission is to bring three electrodes to within 2 nm of each other without short circuits (using mechanical break junction technology and either  $Al_2O_3$  (at Technical University of Delft and at Helmholtzzentrum Rossendorf) or AlN (at the University of Alabama)): no results yet !!!

The second mission would be to synthesize an organic UA molecule with three covalent linkages to three break-junction electrodes (not difficult).

The third mission would be to test whether the UA molecule will work.

The experimental UA project is clearly a many-year mission.

#### ======

- [1] R. M. Metzger, *J. Mater. Chem.* **18**: 4364 (2008).
- [2] R. M. Metzger and D. L. Mattern, Springer Top. Curr. Chem. 313: 39 (2012).
- [3] M. S. Johnson, R. Kota, D. L. Mattern, and R. M. Metzger, "A Two-Faced "Janus" Unimolecular Rectifier Exhibits Rectification Reversal", in preparation.
- [4] A. Honciuc, R. M. Metzger, A. Gong, and C. W. Spangler, J. Am. Chem. Soc. **129**: 8310 (2007)
- [5] C. Toher, D. Nozaki, G. Cuniberti, and R. M. Metzger, *RSC Nanoscale* **5**: 6975 (2013) (funded by the Deutsche Forschungsgemeinschaft).

### Single-molecule electronic components

#### H.S.J. van der Zant

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During the last few years different techniques have become available to study electrical transport through an individual nano-object. These include Au nano-electrodes made with electromigration [1] or fabricated with the mechanically controlled break junction technique [2]. Recently, we introduced graphene [4] as an electrode material for contacting single molecules. With these techniques in place, there is now a shift of focus from the molecule-metal interface [3] to the molecule itself with the goal to exploit the possibilities offered by chemical synthesis and their unique properties such as their large energy level spacings. In this talk I will discuss some examples of this search, which include the use of spin degrees of freedom [5], consequences of quantum interference at room temperature [6] and negative differential resistance devices.

- [1] K. O'Neill, E.A. Osorio and H.S.J. van der Zant, Appl. Phys. Lett. **90** (2007) 133109; F. Prins *et al.*, Appl. Phys. Lett. **94** (2009) 123108.
- [2] C.A. Martin, R.H.M. Smit, H.S.J. van der Zant and J.M. van Ruitenbeek, Nano Lett. **9** (2009) 2940; C.A. Martin, J.M. van Ruitenbeek and H.S.J. van der Zant, Nanotechnology **21** (2010) 265201.
- [3] M. Perrin et al., Nature Nanotechnology 8 (2013) 282.
- [4] F. Prins et al., Nano Letters 11 (2011) 4607.
- [5] H.B. Heersche *et al.*, Rev. Lett. **96** (2006) 206801; E.A. Osorio *et al.*, Nano Lett. **10** (2010) 105; A.S. Zyazin *et al.* Nano Lett. **10** (2010) 3307; E. Burzuri *et al*, Phys. Rev. Lett. **109** (2012) 147203.
- [6] C.R. Arroyo et al., Angewandte Chemie Int. Ed. 52 (2013) 3152.

### Title

### Heike R. Riel

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Abstract

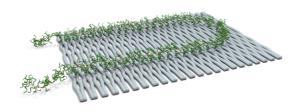


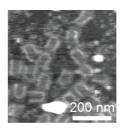
### **DNA-Programmed Assembly of Conjugated Polymers**

Kurt V. Gothelf

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

The idea behind our research is to use 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. We have applied these concepts to assemble and covalently couple conjugated organic molecules<sup>1</sup> and dendrimers.<sup>2</sup> Recently, we extended this to DNA templated conjugation of DNA to proteins. In our studies of DNA origami we have used DNA origami to image chemical reactions with single molecule resolution<sup>3</sup> and to make a 3D DNA origami box with a controllable lid.<sup>4</sup> More recently, we prepared a DNA-phenylene vinylene polymer and assembled it on DNA origami for studies of electronic and optical properties. In extension of this a method for self-assembly of DNA origami and single stranded tile structures at room temperature will also be presented.<sup>5</sup>





Schematic illustration and AFM image of poly(DNA-phenylene vinylene) on DNA origami.

#### References

- 1 Ravnsbæk, J. B et al. Angew. Chem. Int. Ed. 2011, 50, 10851–10854.
- 2 Liu, H. et al. J. Am. Chem. Soc. 2010, 132, 18054-18056.
- 3 Voigt, N. V. et al. Nature Nanotech. 2010, 5, 200-205.
- 4 Andersen, E. S. et al. Nature 2009, 459, 73-76.
- 5 Zhang, Z. et al. Angew. Chem. Int. Ed. 2013 Early View.

### Invited talk abstracts

#### Gianaurelio Cuniberti (TU Dresden)

A bottom-up route to enhance thermoelectric figures of merit in graphene nanoribbons

#### Francesca Moresco (TU Dresden)

STM controlled manipulation of single molecules and molecular structures

**Anton Kiriy** (Leibniz Institute of Polymer Research Dresden)

Controlled polycondensation at work: synthesis of well-defined semiconducting polymers for needs of organic electronics

**Adrian Keller** (Helmholtz-Zentrum Dresden-Rossendorf) *DNA origami-based nanodevices* 

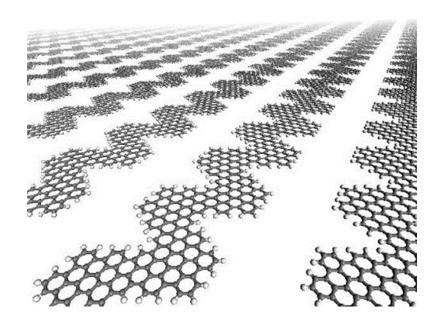
**Jochen Grebing** (Helmholtz-Zentrum Dresden-Rossendorf) *Electronic devices based on nanowires* 

# A bottom-up route to enhance thermoelectric figures of merit in graphene nanoribbons

Gianaurelio Cuniberti<sup>1</sup>, Hâldun Sevinçli<sup>1,2</sup>, Cem Sevik<sup>3</sup>, Tahir Çağın<sup>3</sup>

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We propose a hybrid nano-structuring scheme for tailoring thermal and thermoelectric transport properties of graphene nanoribbons. Geometrical structuring and isotope cluster engineering are the elements that constitute the proposed scheme. Using first-principles based force constants and Hamiltonians, we show that the thermal conductance of graphene nanoribbons can be reduced by 98.8% at room temperature and the thermoelectric figure of merit, ZT, can be as high as 3.25 at  $T=800~\rm K$ . The proposed scheme relies on a recently developed bottom-up fabrication method, which is proven to be feasible for synthesizing graphene nanoribbons with an atomic precision.



#### References

- [1] Cai, J. et al. Atomically precise bottom-up fabrication of graphene nanoribbons. Nature **466**, 470 (2010).
- [2] H. Sevincli et al. A bottom-up route to enhance thermoelectric figures of merit in graphene nanoribbons. Scientific Reports **3**, 1228 (2013).

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# STM controlled manipulation of single molecules and molecular structures

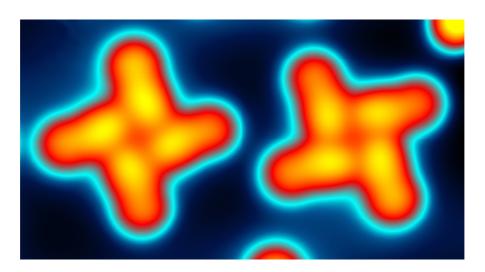
<u>Francesca Moresco</u>, Anja Nickel, Robin Ohmann, Joerg Meyer, Cormac Toher, Lokamani, Dmitry Ryndyk, Gianaurelio Cuniberti

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Low temperature scanning tunneling microscopy (LT-STM) experiments on molecules permit a deeper insight into the quantum electronics of molecular systems and provide important information on the conformational and mechanical properties of single complex molecules. Several methods have been developed in the last years to manipulate molecules using STM, including lateral, vertical, and electrical induced manipulation. In this talk, experiments will be reviewed, where the manipulation process can be controlled by varying one of three main parameters: the electric field, the tunneling current and the forces between tip and surface. In this way, molecules can be exactly positioned on a metal surface and conformational changes can be induced.

Moreover, the electrically controlled manipulation of supramolecular structures will be presented, showing that a structure can be moved collectively in a controlled way. Depending on the applied voltage, several types of movements (translation, rotation, reorganization) of a structure comprised of four 4-Acetylbiphenyl molecules on Au(111) are achieved. By applying consecutive pulses, the structure can be manipulated over larger distances in defined directions. The experiments show a novel possibility to softly and purely electrically manipulate nanostructures on metal surfaces in view of assembly nanoscale devices.



STM image of self-assembled tetramers of 4-Acetylbiphenyl (ABP) on Au(111) ( $\lambda$  and  $\delta$  chiral windmill motif). Image size: 38.4 x 69.3 Å<sup>2</sup>, Bias= -1 V, I=2.9 nA

### Controlled Synthesis of Semiconducting Polymers for Organic Electronics

### Anton Kiriy<sup>1</sup>, Roman Tkachov<sup>1</sup>

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(Semi)conductive/conjugated polymers (CPs) attract considerable attention as promising materials for solar cells, field effect transistors, light-emitting diodes, etc. However, the properties of existing CPs that are prepared predominantly by conventional step-growth polycondensations are still far from optimal. For industrial-scale applications, CPs with controllable molecular weight (MW), MW distribution, chain-end functionality, minimum amounts of defects, and as a result, controlled and reproducible optoelectronic properties are required. In addition, new CP architectures are needed that predictably self-assemble into desirable nanomorphologies, thus solving a longstanding problem with improper morphologies of active layers in heterojunction optoelectronic devices. Nowadays, chain-growth Kumada and Suzuki catalyst transfer polycondensations (KCTP and SCTP, respectively) has become a powerful tool for the synthesis of well-defined conjugated block copolymers, conjugated polymer brushes, 1 endfunctionalized conjugated polymers which are promising materials which might allow a higher degree of morphology control in heterojunction devices. [1,2] This contribution reviews our recent progress in the development of controlled synthesis of conjugated polymers. [3] Especial attention in the lecture will be paid to most recent results obtained in development of controlled chain-growth preparation of electron-deficient (n-type) CPs. particularly, to a novel chain-growth polymerization of a highly unusual anion-radical monomer prepared from 2,6-bis(2-bromothien-5-yl)naphthalene-1,4,5,8-tetracarboxylic-N,N'bis(2-octyldodecyl) diimide (Br-TNDIT-Br) and activated Zn powder. [4,5] Polymerization of this monomer, Br-TNDIT-Br/Zn, in the presence of nickel catalysts led to the corresponding bithiophene-naphthalene diimide conjugated polymer P(TNDT) with controlled molecular weight, relatively narrow polydispersity and specific end-functions (Scheme 1).

#### References:

[1] T. Beryozkina, K. Boyko, N. Khanduyeva, V. Senkovskyy, M. Horecha, U. Oertel, F. Simon, H. Komber, M. Stamm, A. Kiriy. *Angew. Chem. Int. Ed.* **2009**, *48*, 2695.

[2] R. Tkachov, V. Senkovskyy, H. Komber, J.-U. Sommer, A. Kiriy *J. Am. Chem. Soc.* **2010**, *132*, 7803.

[3] A. Kiriy, Senkovskyy, M. Sommer. Macromol. Rapid Commun. 2011, 32, 1503.

[4] V. Senkovskyy, R. Tkachov, H. Komber, M. Sommer, M. Heuken, B. Voit, W. T. S. Huck, V. Kataev, A. Petr, A. Kiriy. *J. Am. Chem. Soc.* **2011**, *133*, 19966.

[5] V. Senkovskyy, R. Tkachov, H. Komber, A. John, J. Sommer, A. Kiriy. *Macromolecules* **2012**, *45*, 4101.

### **DNA** origami-based nanodevices

#### Adrian Keller

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The DNA origami technique<sup>[1]</sup> enables the fast, high-yield synthesis of arbitrarily shaped 2D and 3D nanostructures by exploiting the strong specificity of Watson–Crick base pairing. It employs a long, single-stranded DNA scaffold which is folded into the desired shape by a suitable (*i.e.*, complementary) set of designed short synthetic oligonucleotides, called staple strands. The sequence of each staple strand is designed to facilitate multiple binding events with different segments of the scaffold strand, thus forcing the scaffold to fold into an arbitrary shape which is determined by the sequences of the individual staple strands. Each staple strand can be extended to protrude from the DNA origami surface, resulting in a well-defined DNA system with more than 200 individually addressable sites that are located ≥ 4 nm apart from each other. The selected protruding strands can be modified systematically with respect to length, nucleobase sequence, and hybridization state, and synthesized to carry various chemical modifications. In this way, "molecular breadboards" can be realized that enable the controlled arrangement of functional entities such as metal nanoparticles (see Fig. 1), quantum dots, fluorophores, carbon nanotubes, and various proteins. [2]

This talk will provide an overview of our recent activities focused on the fabrication of functional DNA origami-based nanodevices with potential applications in structural biology, molecular sensing, and nanoelectronics.

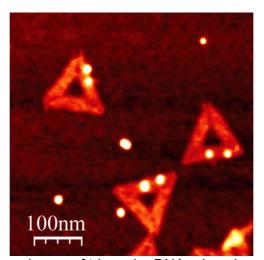


Fig.1: Atomic force microscopy image of triangular DNA origami nanostructures carrying two 5 nm gold nanoparticles.

#### References:

- [1] P. W. K. Rothemund, *Nature* **2006**, *440*, 297-302.
- [2] T. Tørring, N. V. Voigt, J. Nangreave, H. Yan, K. V. Gothelf, *Chem. Soc. Rev.* **2011**, *40*, 5636-5646.

### **Strategies for Contacting Single Molecule Devices**

Matthias Wieser<sup>1</sup>, Torsten Sendler<sup>1</sup>, Filip Kilibarda<sup>1</sup>, Bezuayehu Teshome<sup>1</sup>, Adrian Keller<sup>1</sup>, <u>Jochen Grebing</u><sup>1,2</sup>, Artur Erbe<sup>1</sup>

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Single molecules have been under investigation in terms of their suitability as building blocks for future electronics for more than a decade now. But the ultimate goal of molecular electronics is the (controlled) creation of functional electric circuits, i.e., networks, rather than individual devices. This requires two aspects to be addressed: The properties of the devices themselves and the properties of the contacts between individual devices as well as to the molecules forming the devices.

Traditionally, top-down methods are used to form these contacts. Here, results of measurements on PEEB (P-Ethoxy Ethyl Benzoate) molecules using the technique of mechanically controllable break junctions will be presented.

However, a bottom-up approach is favorable because of the reduced effort in fabrication. Therefore, in the second part an intermediate, hybrid approach using DNA double helix bundles as templates for leads and top-down fabricated contacts to establish a connection to the macroscopic world will be discussed.

#### Poster abstracts

- **T. Sendler**, M. Wieser, J. Wolf, T. Huhn, E. Scheer, F. Moresco, J. Grebing, A. Erbe *Electrical characterization of single organic molecules via mechanically controllable break junctions*
- **D. Deb**, M. Helm, A. Erbe , J. Grebing Development of gated single molecule contacts using reconfigurable SiNWs (by Top-Down Process)
- **E. Baek**, S. Pregl, L. Römhildt, L. Baraban, G. Cuniberti *Optical Gating of Porphyrin-covered Si Nanowire FETs*
- **Y. Aleksandrov**, C. Fowley, K. Bernert, V. Sluka, E. Kowalska, M. Farle, J. Lindner, B. Ocker, J. Fassbender, A. M. Deac *Ferromagnetic resonance of perpendicular magnetic anisotropy MgO/CoFeB based tri-layers*
- J. Kelling, S. Gemming

Ab-initio investigation of carbides and of CNT junctions at finite temperature and under stress

**Lokamani**, A. Nickel, J. Meyer, R. Ohmann, D. Ryndyk, F. Moresco, G. Cuniberti *Pulse-induced switching of acetylbiphenyl on silicon* 

- **B. Teshome**, S. Facsko, A. Keller *Topography-controlled alignment of DNA origami nanotubes on nanopatterned surfaces*
- **G. Öktem**, A. Kiriy, R. Jordan Thiophene bearing well defined semiconducting oligomers along with thiol anchoring groups: synthesis and thickness measurements
- **J. F. Nawroth**, R. Jordan, S. Diez Surface patterning and positioning of tPads on the nanoscale
- **M. Hetti**, M. Bartusch, B. Voit, D. Pospiech Synthesis and characterization of functionalized magnetic nanoparticles
- **B. lyisan**, J. Kluge, D. Appelhans, B. Voit Functional polymersomes designed for covalent and non-covalent conjugation

# Electrical characterization of single organic molecules via mechanically controllable break junctions

<u>Torsten Sendler</u><sup>1</sup>, Matthias Wieser<sup>1</sup>, Jannic Wolf<sup>2</sup>, Thomas Huhn<sup>2</sup>, Elke Scheer<sup>2</sup>, Francesca Moresco<sup>3</sup>, Sibylle Gemming<sup>1</sup>, Jochen Grebing<sup>1</sup>, Artur Erbe<sup>1</sup>

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Molecular electronics has been a field of big interest for the last years. Using the technique of mechanically controllable break junctions we characterize different organic molecules, e.g. 1,4-Diethoxy-2,5-bis(4-sulfanyl-phenylethynyl)-benzene (PEEB) and switchable molecular wires, dissolved in an organic non-polar solvent. IV-curves taken from the molecules connected to single gold atom contacts show the expected tunneling behavior described by the single-level model: weak coupling of the molecules to the gold atoms implies an off-resonant tunneling process and a transport through a single channel. Varying the end-groups of the molecules leads to a different transport behavior. Figure 1 shows a 2D histogram of IV-curves of PEEB with amino end-groups. Based on the single-level transport model the analysis of the current-voltage characteristics delivers the energy of the molecular level and the coupling between electrode and molecule. It also indicates a reliable contact of the molecules to the gold atoms. A further goal is the investigation of an electric gate effect on the transport behavior through the molecules.

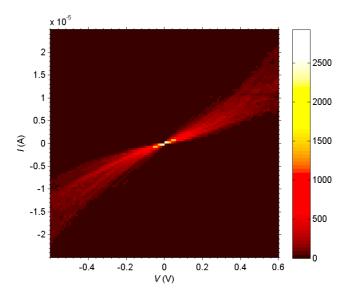


Fig. 1: 2D histogram of IV-curves of PEEB with amino end-group

# Development of gated single molecule contacts using reconfigurable SiNWs (by Top-Down Process)

D. Deb<sup>1,2</sup>, M. Helm<sup>1,2</sup>, A. Erbe<sup>1</sup>, J. Grebing<sup>2</sup>

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Single molecules have individual electronic properties which offer a wide range of components for molecular electronics [1]. Moreover these components are flexible and bio-compatible [2, 3]. Recent experimental advancements reveal that molecular electronics has the potential to be the next generation transistor component [1].

In this project we put forward a new idea of silicon compatible and gate controlled molecular junctions. We intend to fabricate undoped silicon nanowire (SiNW) by Top-Down process on SOI wafers with electron beam lithography followed by controlled silicidation of the silicon nanowires (SiNW) to achieve atomic sharp Si-NiSi<sub>2</sub> interfaces at the center. After successfully fabricating the nanowires we will cover it with HfO<sub>2</sub> by ALD process followed by metallization to form gates. These devices should be able to work as p-FET as well as n-FET (reconfigurable device) [4].

For characterization steps we will use the mechanically controllable break junction (MCBJ) technique [1, 2] at ultra-high vacuum (UHV) condition or inert liquid atmosphere. Application of controlled stress is expected to break the silicon nanowire (SiNW) with high precision and we can introduce a single molecule between the two contacts to form Si-Molecule-Si channel. This will enable us to do transport measurements through individual molecules. As far as molecules are concerned, we will start with –OH anchoring groups due to oxyphilic behavior of Si [5]. The main alkene or aromatic chain of the molecule can be doped by adding different side groups [3, 6].

At the molecular contacts, alignment of the energy levels (of molecule and contact) is an important factor for resonant transport [1]. To control the charge injection through the contact (and control the energy levels) we will like to use external gate biasing. By using reconfigurable silicon nanowire (SiNW) we can control the charge injection (hole or electron) through the molecular contact and achieve highly tunable junctions.

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# **Optical Gating of Porphyrin-covered Si Nanowire FETs**

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We study optical gating process of porphyrin-coated silicon nanowire field effect transistors (Si NW FETs) which shows switching of current under light illumination.

Porphyrin, which is the organic pigment molecule, absorbs broad range of visible light and easily transfers energy and electrons to other molecules or inorganic backbone due to its conjugated ring structure. Si NW based FET containing nickel silicide Schottky barriers have been fabricated by bottom-up way, and functionalized by porphyrin molecules to explore the possibility to gate nanowire based devices by light.

Here we propose new mechanism of optical switching of devices by molecular polarization of porphyrin layer. Polarized porphyrin layer acts as top gate of the device, which induces charge carriers in NW channels. Also, we demonstrate that optoelectrical current-switching highly depends on porphyrin concentration. Switching time constant is extracted using exponential growing and decaying function and be compared by the thickness of porphyrin layer. As the concentration increases, the devices show fast switching due to low resistance of porphyrin. Switching on/off ratio by light is reduced when the porphyrin layer is too thick to conduct the light irradiation. Understanding the electrical charging mechanism between molecules and NWs will facilitate the systematic integration of the molecular hybrid devices.

# Ferromagnetic resonance of perpendicular magnetic anisotropy MgO/CoFeB based tri-layers

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Magnetic tunnel junctions with perpendicular magnetic anisotropy (PMA) are good candidates for next generation spin-transfer-torque magnetic random access memory (STT-MRAM) [1]. Besides a comparatively higher thermal stability than in-plane MA, the recently reported appearance of PMA in MgO/Co<sub>40</sub>Fe<sub>40</sub>B<sub>20</sub>/Ta structures allows for lower switching currents while maintaining high quality MgO barrier growth.

In this report we use the ferromagnetic resonance technique to investigate the magnetic properties of a CoFeB layer sandwiched by Ta and MgO layers. Samples were grown by RF or DC sputtering using a TIMARIS cluster deposition tool (Singulus Technologies AG) [2] and annealed in  $N_2$  environment for 30 minutes at temperatures between 150 and 250°C in steps of 50°C. FMR measurements are performed at room temperature using a microwave cavity [3]. Thin films are also investigated by standard magnetometry measurements in a SQUID/VSM and also by the extraordinary Hall effect to extract the saturation magnetization and effective anisotropy.

Through FMR we are able to simultaneously extract the out-of-plane anisotropy, the effective magnetization and the damping co-efficient, as a function of annealing temperature. Our results show that post-annealing systematically shifts the magnetic easy axis from in-plane to out-of-plane direction. As the annealing temperature is increased the effective magnetization also increases.

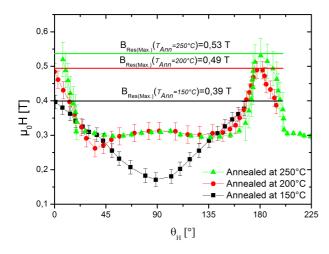


Figure 1: FMR resonance field as a function of polar angle. At  $\theta_H$ =0 field is parallel to the film plane. The increase in the resonance field in the film plane indicates that, with higher annealing temperatures, the magnetization easy axis turns more into the out-of-plane direction.

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# Ab-initio investigation of carbides and of CNT junctions at finite temperature and under stress.

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With the presented work we lay the foundation for ab-initio studies of contacted carbon nanotubes with both metal and metal--carbide leads. We focuson applying the frozen phonon method on top density-functional-theory calculations for electronic the system. Here we show our ab-initio results on the elastic and electronic properties of Al<sub>4</sub>C<sub>3</sub> and the metastable Ni<sub>3</sub>C.

Furthermore we present an alternative non-perturbative approach to calculating the quantum conductance in CNT/molecular junctions at finite temperature. Strictly employing the Born--Oppenheimer approximation, we aim to calculate the influence of phonons on the conductance of such a system by averaging over a representative sample drawn from snapshots of thermal fluctuation of the lattice.

# Pulse-induced switching of acetylbiphenyl on silicon

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Owing to the advances in nano-scale miniaturisation of conventional silicon-based technology according to "Moore's Law", the lateral feature sizes of integrated electronic devices are currently in the range of few tens of nanometers [1]. Further advancements in nano-scale minaturistation are going to pose constraints on the existing design rules and fabrication technology, mainly due to physical limitations like e.g. lateral tunneling between devices [2]. Henceforth a new trend "More that Moore" has emerged in the past few years focusing on diversification of integrated devices rather than sole miniaturisation [1].

Nanoelectromechanical systems (NEMS) [3-4], which are usually comprised of single molecules sandwiched between metal electrodes and are characterized by strong coupling of electronic and mechanical degrees of freedom, could act as a complementing devices in extending the functionality of the existing silicon-based technology. Due to the strong coupling, reversible conformational changes can be induced in the NEMS using current or voltage impulses and the conformational associated transfer characteristics can be exploited to perform computation or store information.

One of the possible candidates which could act as a NEMS is the organic molecule Acetybiphenyl. Acetybiphenyl is comprised of two benzene rings and an acetyl-functional group. Acetylbiphenyl shows interesting switching properties on silicon (100) surface. It can switch between two stable configurations back and forth when a voltage pulse is applied to the adsorbed molecule using the tip of a scanning tunneling microscopy (STM). Together with atomic-scale wires formed by silicon dangling bonds [2], it would be possible to design logic circuits using just acetybiphenyl-like molecules.

Here we investigate in a joint experiment-theory effort the possible switching mechanism of acetybiphenyl on Si(100) surfaces and possible uses of such molecules in logic circuits.

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# Topography-Controlled Alignment of DNA Origami Nanotubes on Nanopatterned Surfaces

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Since its discovery, the DNA origami technique<sup>1</sup> has attracted considerable attention from various research fields. By this technique, it has become possible to generate complex 2D and 3D DNA nanostructures with any desired shape. Quasi-one-dimensional DNA nanostructures hold particularly great promise as scaffolds for nanoelectronic device fabrication. However, the fabrication of functional nanoelectronic devices from such DNA nanostructure templates requires their controlled arrangement and orientation on a conventional substrate. In the past, various techniques have been employed to control the alignment of immobilized DNA nanostructures on different surfaces<sup>2,3</sup>. However, most techniques rely on lithographic prepatterning and often also a chemical functionalization of the substrate.

In this work, we demonstrate a compelling alternative approach to generate ordered arrays of DNA nanotubes on topographically patterned surfaces. To this end, we combine two bottom-up techniques for nanostructure fabrication, i.e., DNA origami self-assembly and self-organized nanopattern formation on silicon surfaces during ion sputtering<sup>4</sup>, thus avoiding the necessity of lithographic processing or chemical modifications. The self-alignment of the six-helix-bundle (6HB) DNA origami nanotubes is purely driven by electrostatic interactions with the nanorippled  $Si/SiO_2$  surface during adsorption. By tuning the pattern dimensions to match the dimensions of the DNA origami nanotubes, we obtain an alignment yield of  $\sim 70\%$ .

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# Thiophene bearing well defined semiconducting oligomers along with thiol anchoring groups: synthesis and thickness measurements

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π- Conjugated molecules are critical components of molecular electronics since they provide the control of the tunneling of electrons via synthetic chemistry. The influence of molecular structure on electrical conductance properties is investigated by integrating conjugated molecules in metal-molecule-metal junctions. Accordingly, the standing-up phase of conjugated molecules should be very well defined in order to integrate molecule definitely in between these two metal electrodes, not to be flatly adsorbed on electrode surface. For this purpose, in this study, the positioning of conjugated molecules on gold surface is aimed to be defined as a result of thickness measurements. In this study, Surface-Initiated Kumada Catalyst-Transfer Polycondensation is utilized for the controlled synthesis of thiophene bearing semiconducting oligomers in different conjugation lengths. The first generation of thiophene related well defined oligomers both possessing single/double-sided thiol end-groups and benzene/biphenyl substituents between oligomer backbone and anchoring groups are synthesized.

The positioning of sulfur containing single molecules adsorbed on a gold surface is investigated via Surface Plasmon Resonance Spectroscopy (SPR) and/or in-situ Ellipsometry. By means of the thickness of layers formed by standing-up or stacked/unstacked lying-down alignments on Au surface, the effect of thiophene bearing oligomers on positioning and thickness is investigated by comparing with bare benzenethiol/biphenylthiol containing surfaces. Additionally, the possibility of interaction between gold and thiophene-sulfur is eliminated or proven and can be prevented by covering a shell around thiophene for further applications. This study reveals preliminary point of view for single molecule conductance studies through Mechanically Controllable Break Junctions (MCBJs).

# Surface Patterning and Positioning of tPads on the Nanoscale

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One way to further improve the performance of computers is to decrease the size of the structures on the wafers. Recent production standards use top-down methods that are mainly limited by the wavelength of the light that is used to irradiate the masks and to develop the resists.

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 (tPads) but the challenge for this very project is to pattern the Si-based substrate in a way that the tPads 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 5nm. The generated structures are carbon deposits that can be used for further functionalization.

Self-initiated photografting and photopolymerization (SIPGP) uses the proton abstraction from the surface that occurs with vinyl monomers under UV-irradiation. This generates surface bound radicals that lead to polymer brushes growing from the surface. However, this does not work on bare Si since the Si-H bonding dissociation energy is too high, 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 tPad on the substrate but also, depending on the used monomer, the binding affinity to the brush.

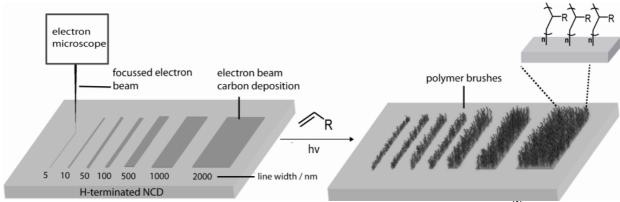


Figure 1 - Preparation of structured polymer brushes on diamond with electron beam lithography<sup>[1]</sup>

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# Synthesis and Characterization of Functionalized Magnetic Nanoparticles

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Magnetic nanoparticles were synthesized and surface functionalized. Firstly, magnetite nanoparticles (Fe<sub>3</sub>O<sub>4</sub> NP) were synthesized by precipitating ferrous and ferric chlorides with ammonium solution. The resultant purified nanoparticles form stable dispersion in ethanol with little aggregation and have an overall 151 nm of mean hydrodynamic diameter. Transmission electron micrographs (TEM) observe that Fe<sub>3</sub>O<sub>4</sub> NP was about 10 – 25 nm in diameter in dried state. Moreover, they also contain surface hydroxyl groups for further surface modification. The nanoparticles were then surfaced functionalized by two approaches. In the first approach, Fe<sub>3</sub>O<sub>4</sub> NP was modified with oleic acid by physical adsorption to form oleic acid modified magnetite nanoparticles (Fe<sub>3</sub>O<sub>4</sub>-OA). The resultant nanoparticles form a very stable dispersion in toluene with mean hydrodynamic diameter of about 68 nm. Scanning electron micrographs (SEM) show that Fe<sub>3</sub>O<sub>4</sub>-OA can stick well and evenly distributed on ultra high molecular weight polyethylene woven fabrics' surface. In the second approach, the Fe<sub>3</sub>O<sub>4</sub> NP was modified with α-bromo isobutyryl bromide (BIBB) to form BIBB modified magnetite nanoparticles (Fe<sub>3</sub>O<sub>4</sub>-BIBB NP) with covalent linkages. The resultant Fe<sub>3</sub>O<sub>4</sub>-BIBB NP will be used as a macroinitiator for atom transferred radical polymerization (ATRP). The functionalized nanoparticles will incorporate with polymers and high performance fibres and will be applied in the field of health monitoring.

# Functional polymersomes designed for covalent and non-covalent conjugation

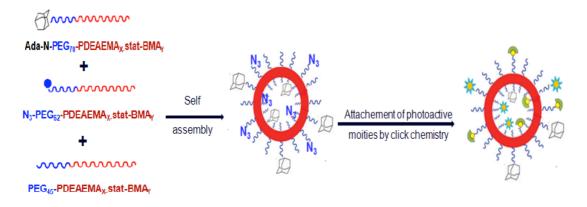
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Polymersomes are class of artificial vesicles that is composed of amphiphilic block copolymers in an aqueous environment. They resemble liposomes in their architecture, but have some additional properties. They are more stable and more prone to chemical functionalization compared to liposomes<sup>1</sup>. Thus, they have promising applications including targeted drugdelivery systems, biosensors, nanoreactors or synthetic organelles. For all these applications, block copolymer membrane has played an important role since its interaction with the surroundings of polymersome system determines the potential biomedical applications. By altering the surface of the polymersomes, it is possible to attach some molecules such as antibodies, enzymes, or photoactive moieties to the shell of polymersome<sup>2</sup>.

The main concern of this study is to prepare photoactive polymersomes, including their non-covalent attachment onto surfaces, which can be used as carrier systems or biosensors in biomedical field. In order to reach this aim, here, we report the synthesis of functional polymersomes which have photoactive and/or adamantane (Ada) groups at their periphery. As the base of our study, we first synthesized amphiphilic *PEG-b-P(DEAEMA-stat-BMA)* block copolymer via atom transfer radical polymerization (ATRP)<sup>3</sup>. Secondly block copolymers, possessing azide or Ada end groups, were synthesized via ATRP. By self assembly of these various amphiphilic block copolymers in aqueous solution, various stable functionalized polymersomes were established. The intensity-average diameter of polymersomes was in the range of 120-150 nm and determined by dynamic light scattering (DLS). Further functionalization of these polymersomes to attach photoactive moties to the polymersome periphery were performed by using click chemistry. Additionaly, to prove non-covalent interactions in the polymersomes' shell, host-guest interactions between Ada-modified polymersomes and cyclodextrin modified molecules were monitored by using UV-Vis spectroscopy.



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