

International Helmholtz Research School  
for Nanoelectronic Networks

# IHRS NANO NET Annual Workshop 2017

16 – 18 August 2017

Hotel Neue Höhe, Klingenberg, Germany



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## Venue and organization

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## NanoNet Annual Workshop 2017, Klingenberg

### Talks

updated: 14.08.2017 (PZ)

Presenter	No.	Title	Pg.
<b>Invited Talks</b>			
Jordan, R.		From Self-assembled Monolayers to Polymer Brushes	2
Lissel, F.		Towards Organometallic Electronics: Metal-Ligand Systems in Molecular and Polymer Electronics	3
Metzger, R.M.		The Smallest Unimolecular Rectifier, Coulomb Blockades & Other Results	4
Samano, E.		Self-organization of inorganic material <i>via</i> DNA nanostructures	5
Tornow, M.		Self-assembled monolayers as model systems for studying charge transport at organic-inorganic interfaces	6
<b>Contributed Talks</b>			
Bayrak, T.	T4	Functionalized DNA Origami Nanostructures for Molecular Electronics	7
Fuchs, F.	T2	Simulation of Reconfigurable Field-effect Transistors: Impact of the NiSi <sub>2</sub> -Si Interfaces, Crystal Orientation, and Strain	8
Kelling, J.	--	Efficient Parallel Monte-Carlo Simulations for Large-Scale Studies of Surface Growth Processes	9
Khan, M.B.	T1	Performance Enhancement of Reconfigurable Field Effect Transistors	10
Skidin, D.	T5	On-surface polymerization of donor-acceptor-donor molecules	11
Ye, J.	T3	Nano-electronic components built from DNA templates	12

List of Poster Contributions see list on page 13.

# From Self-assembled Monolayers to Polymer Brushes

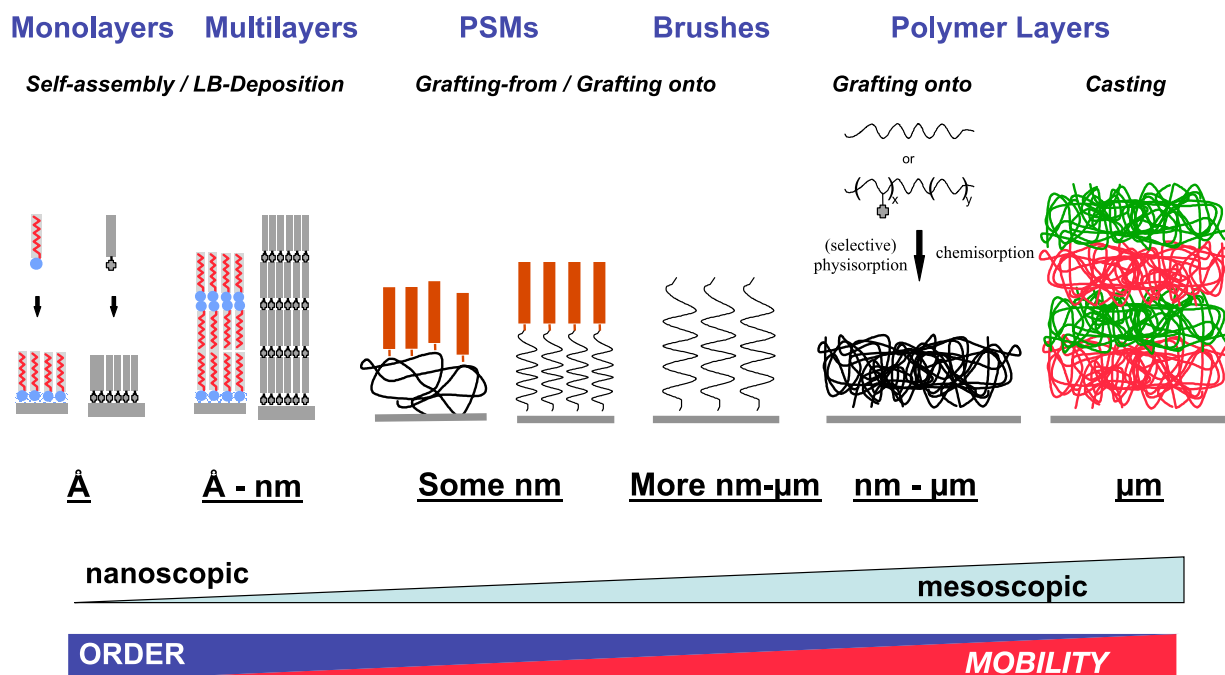
Rainer Jordan

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This tutorial lecture will give a brief overview on the preparation and properties of self-assembled monolayers (SAMs) and their use as two-dimensional initiator systems for the preparation of polymer brushes by means of surface-initiated polymerization (SIP) including free radical, controlled radical, living ionic and other polymerizations. Recent advances in the preparation of defined surface coatings with programmed heterogeneities such as micro- and nanopatterned as well as graded surfaces will be summarized.

Beside the standard surface coupling chemistry using silanes or thiols for oxides and coin metals, alternative chemistry suitable for other substrate materials such as carbon based materials (e.g. graphene, diamond, silicon carbide) will be presented. As time allows, I will also give an example of a "surface modifications without a substrate".



# **Towards Organometallic Electronics: Metal-Ligand Systems in Molecular and Polymer Electronics**

Dr. sc. nat. Franziska Lissel

Leibniz Institute for Polymer Research Dresden, Germany

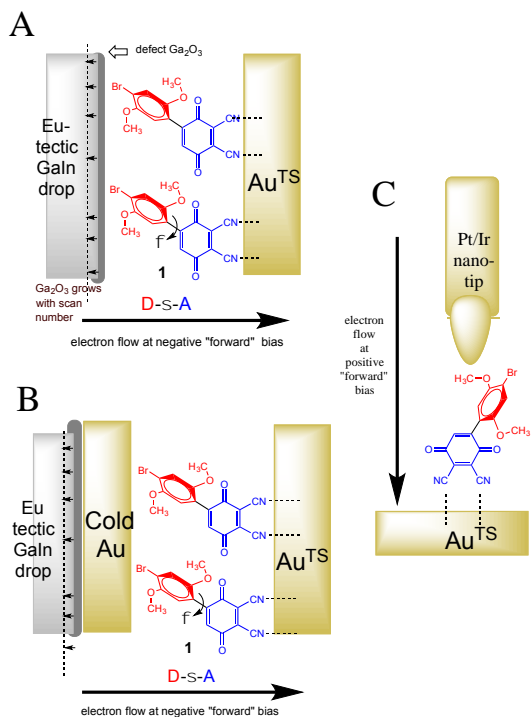
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The vision of molecular electronics is to employ molecules as passive and active building blocks in electronic circuits. This requires the design and realization of molecules which (a) show high charge transport rates, (b) are functional and react to external stimuli, and (c) bind mechanically stable to electrodes. Currently the focus is on organic molecules, yet their molecular orbitals (MO) and the Fermi Level ( $E_F$ ) of the common metal electrodes are usually separated by several eV, and creating functionality requires synthetically challenging and spatially extensive architectures. Organometallic molecules are an interesting alternative, as their MO energies are closer aligned to  $E_F$  and can be easily tuned using different metal centers and ligands. The covalent insertion of early transition metals in the charge conductance pathway also makes their intrinsic redox and spin functionality directly accessible while maintaining utmost structural density.

A common problem encountered in the field of polymer-based organic electronics is the vulnerability of fabricated devices to mechanical stress caused by thermal expansion, bending and stretching. These different types of mechanical stress lead to a loss of electronic performance and ultimately the failure of the device. Previous breakthroughs in stretchable and durable electronics stem from strain engineering and nanocomposite approaches. The molecular approach, i.e. creating materials that are intrinsically stretchable and resilient to mechanical strain, would enable mechanically robust devices by simple fabrication processes such as direct printing and coating, and contribute to new application areas such as biocompatible and skin-inspired electronics. The realization of intrinsically stretchable materials requires the introduction of dynamic bonds that can reversibly break and re-form under mechanical stress. Non-covalent bonds such as metal-ligand interactions are a promising option, as they allow extensive tuning of the bonding strength and the resulting mechanical properties.

# The Smallest Unimolecular Rectifier, Coulomb Blockades & Other Results

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**(One) HBQ** is a twisted hemibiquinone (weak electron donor + weak electron acceptor with a large intramolecular twist angle  $\phi \approx 35^\circ$ ); it is only 1.1 nm long [1]. HBQ chemisorbs onto Au. The DC electrical current is asymmetric, because HBQ rectifies in the "reverse Aviram-Ratner direction". The rectification ratios (RR) are RR=150 to 200 at 2.5 Volts when studied **(A)** as a monolayer between Au and an eutectic GaIn drop; this RR grows upon repeated scans because an interfacial  $\text{Ga}_2\text{O}_3$  thickens. When an **HBQ** monolayer is measured between Au and cold Au **(B)** then RR is smaller, RR=5 to 40 at 2.5 Volts. When a **single HBQ molecule** is measured by scanning tunneling spectroscopy **(C)** between Au and a PtIr nanotip, RR=3 to 8 at 1.5 Volts. HBQ is the

smallest known significant rectifier [1], and **(D)** work in Singapore confirmed RRs of the order of 150 with excellent statistics when using an GaIn top electrode directly (no cold Au) [2]. NEGF calculations (TranSIESTA) for **HBQ** between Au electrodes are underway [3]: we hope to confirm the rectification.

**(Two)** No current is seen for a TMPD-perylenebisimide rectifier monolayer between  $\pm 1$  Volts (Coulomb blockade at 300 K) [4].

**(Three)** The conditions for 3D metallic behavior for top cold Au pads were established (2 x 2 g Au pellets are evaporated to make 35 nm thick cold Au pads) [5].

**(Four)** Experiments for a theoretically predicted unimolecular power amplifier [6] are unfunded and very difficult.

[1] J. E. Meany, M. S. Johnson, S. A. Woski, & RMM, *ChemPlusChem* **81**, 1152 (2016).

[2] C. A. Nijhuis, unpublished results.

[3] C. L. Horton and RMM, in preparation.

[4] M. S. Johnson, R. Kota, D. L. Mattern, and RMM, *Langmuir* **32**, 685 (2016).

[5] M. S. Johnson, C. L. Horton, M. R. A. Monnette, and RMM, in revision.

[6] C. Toher, D. Nozaki, G. Cuniberti, and R. M. Metzger, *Nanoscale* **5**, 6975 (2013).

## Self-organization of inorganic material *via* DNA nanostructures

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Nowadays there is an intensive search for nanomaterials to be applied towards novel emerging nanodevices. Artificial DNA nanostructures such as DNA origami have garnered significant interest as templates for organizing materials because their design allows for the incorporation of binding sites to assemble nanocomponents with 5 nm resolutions. The DNA origami strategy for assembling designed supramolecular complexes requires ssDNA as a scaffold strand. A system is described that was designed using approximately one third of the M13 bacteriophage genome as a scaffold. Folding of the short 2404-base ssDNA scaffold into a variety of two-dimensional origami shapes with high assembly yields is demonstrated. The nanostructures have minimum size but identifiable geometry. DNA origami templates, modified to have DNA binding sites with a uniquely coded sequence can be used to produce complex metallic nanostructures of programmable design. Gold nanoparticles functionalized with a complementary DNA sequence were attached to specific binding sites in a highly controllable to form a predesigned array on two nanostructures. Finally, the use of an artificial, diblock polypeptide with affinity for DNA in the stabilization of DNA origami and DNA-functionalized gold nanoparticles in solution is discussed. The aim is to expand bionanomanufacturing strategies for solution phase fabrication of photonic and electronic devices.

# Self-assembled monolayers as model systems for studying charge transport at organic-inorganic interfaces

Marc Tornow

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Molecular self-assembled monolayers (SAMs) on inorganic substrates – particularly on semiconductors - have gained importance as functional interfaces for applications in sensing, organic electronics and energy conversion. Understanding electronic charge transport in and across these nanometer-thick coatings is essential, for tailoring and predicting the function of devices.

I will present our recent work on various aliphatic and aromatic organophosphonate SAMs grown on silicon oxide<sup>1-2</sup> and alumina<sup>3-4</sup>, focusing on their dielectric, and in particular on their electronic charge transport properties: While the conductance through simple alkane phosphonates follows an expected non-resonant tunneling characteristic at low bias, their analog bis-phosphonate SAMs reveal an intriguingly strong damping of tunneling currents. This behavior can be attributed to electron tunneling paths known from models that describe charge transfer in highly complex systems such as proteins.

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2. Cattani-Scholz, A.; Liao, K. C.; Bora, A.; Pathak, A.; Hundschell, C.; Nickel, B.; Schwartz, J.; Abstreiter, G.; Tornow, M., Molecular Architecture: Construction of Self-Assembled Organophosphonate Duplexes and Their Electrochemical Characterization. *Langmuir* **2012**, 28, 7889–7896.
3. Pathak, A.; Bora, A.; Liao, K. C.; Schmolke, H.; Jung, A.; Klages, C. P.; Schwartz, J.; Tornow, M., Disorder-derived, strong tunneling attenuation in bis-phosphonate monolayers. *Journal of Physics Condensed Matter* **2016**, 28 (9), 094008.
4. Pathak, A.; Bora, A.; Braunschweig, B.; Meltzer, C.; Yan, H.; Lemmens, P.; Daum, W.; Schwartz, J.; Tornow, M., Nanocylindrical confinement imparts highest structural order in molecular self-assembly of organophosphonates on aluminum oxide. *Nanoscale* **2017**, 9, 6291-6295.



# Functionalized DNA Origami Nanostructures for Molecular Electronics

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The DNA origami method provides a programmable bottom up approach for creating nanostructures of any desired shape, which can be used as scaffolds for nanoelectronics and nanophotonics devices. This technique enables the precise positioning of metallic and semiconducting nanoparticles along the DNA structures. In this study DNA origami nanotube and mold chains are used for the fabrication of gold nanowires. To that end, electroless gold deposition is used to selectively grow the gold nanoparticles (AuNPs) and create eventually continuous nanowires. In order to investigate the transport properties of the individual DNA origami based metallic wires, electrical contacts are developed by electron beam lithography. Current-voltage measurement of along wires at room temperature shows that they all have ohmic behavior. Resistances of DNA origami based wires are in the range of 87ohm to 28Gohm for 90 nm to 1µm length wires. Conductivity of wires is increased by introducing bis-end thiolate functionalized oligo (3-hexylthiophene) molecule between the gap (7nm) of grown nanoparticles. Additionally, the assembly of heterogeneous nanostructures, i.e. AuNPs and semiconductor quantum dots (QDs), on a single DNA origami nanotube is demonstrated and further metallized, thus representing a first step toward the future fabrication of DNA origami-templated quantum dot transistors.

# **Simulation of Reconfigurable Field-effect Transistors: Impact of the NiSi<sub>2</sub>-Si Interfaces, Crystal Orientation, and Strain**

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Reconfigurable field effect transistors (RFETs) can be switched between electron and hole current by changing the polarity of the gate potential. The device performance of such a transistor is strongly dominated by the contact physics.

In this work, the electron transport across the NiSi<sub>2</sub>-Si interface is studied using the NEGF formalism and density functional theory. A new model is presented which relates the electron transport through the interface to the transfer characteristic of an RFET. The model is compared to experimental data showing good agreement.

Based on the model, the influence of strain and the choice of the crystal orientation is discussed. It is demonstrated that best symmetry between electron and hole current is achieved for the <110> orientation. Furthermore, this symmetry can be tuned by strain, which is not possible for the <100> and <112> orientations. A discussion of these differences based on band structure analysis will be given, too.

# Efficient Parallel Monte-Carlo Simulations for Large-Scale Studies of Surface Growth Processes

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Géza Ódor<sup>3</sup>, Martin Weigel<sup>4</sup>, Sibylle Gemming<sup>2,5</sup>

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Lattice Monte Carlo methods are used to investigate far from and out-of-equilibrium systems, including surface growth, spin systems and solid mixtures. Such studies require observations of large systems over long times scales, to allow structures to grow over orders of magnitude, which necessitates massively parallel simulations. This talk presents work done to address the problem of parallel processing introducing correlations in Monte Carlo updates. Studies of the effect of correlations on scaling and dynamical properties of surface growth systems and related lattice gases is investigated further by comparing results obtained by correlation-free and intrinsically correlated simulations. Where the latter, based on a stochastic cellular automaton approach, are of interest because of their high efficiency. The primary subject of study is the Kardar–Parisi–Zhang surface growth in (2+1) dimensions. Key physical insights about this universality class, like precise universal exponent values and exponent relations, obtained from large-scale simulations are presented.

At the end of the talk, I will also speak about my current work at the computational science group at HZDR, which includes problems like frameworkdevelopment, image analysis and related machine learning applications.

# Performance Enhancement of Reconfigurable Field Effect Transistors (RFETs)

Muhammad Bilal Khan<sup>1</sup>, Dipjyoti Deb<sup>1,2</sup>, Yordan M. Georgiev<sup>1</sup>, Artur Erbe<sup>1,2</sup>

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Scaling down of CMOS faces strong challenges due to which advanced fabrication techniques, advanced materials, new device and logic concepts have gained importance. These concepts include undoped silicon nanowire based reconfigurable devices, which can be programmed as *p*- or *n*-channel FETs by controlling the electrostatic potential applied at gate electrodes. In this talk, fabrication and electrical characterization of undoped sub-20 nm silicon nanowires (SiNWs) will be reported. SiNWs are fabricated on intrinsic silicon-on-insulator (SOI) substrates in <110> and <100> crystal orientations using a top down approach. Hydrogen silsesquioxane (HSQ), a negative tone electron beam resist, is used for nano-patterning and as a hard mask for etching. Nanowire etching process is optimized using an inductively coupled plasma (ICP) source and C<sub>4</sub>F<sub>8</sub>/SF<sub>6</sub>/O<sub>2</sub> mixed gas recipe at 18 °C. These NWs are subsequently silicidized to form Schottky junctions. Electrical characterization shows different charge carrier transport in <110> and <100> crystal orientations. Control over silicide formation to enhance the performance of these devices will be discussed.

## On-surface polymerization of donor-acceptor-donor molecules

Dmitry Skidin<sup>1</sup>, Tim Erdmann<sup>2,3</sup>, Frank Eisenhut<sup>1</sup>, Justus Krüger<sup>1</sup>, Anton Kiriya<sup>2,3</sup>,  
Brigitte Voit<sup>2,3</sup>, Francesca Moresco<sup>1,2</sup>, and Gianaurelio Cuniberti<sup>1,2</sup>

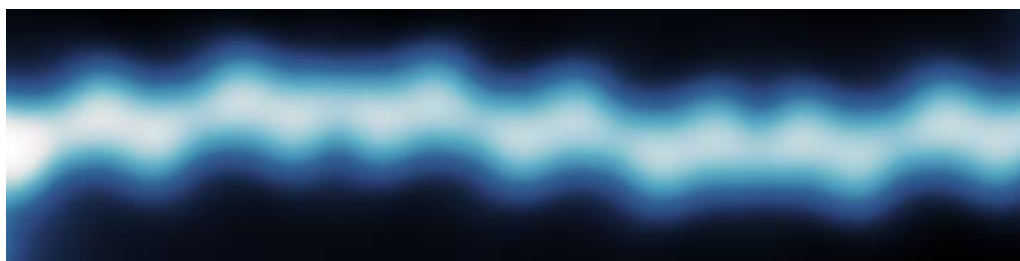
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The key step towards realization of molecular-scale electronics is a search of the new molecular materials with enhanced electronic properties. Specifically, molecular wires with high conductance could be employed as functional units for the circuitry at nanoscale. Here, we demonstrate on-surface polymerization of donor-acceptor-donor molecules into highly conductive molecular wires. An approach of combining donor and acceptor groups in one molecule (polymer) is inherited from organic photovoltaics where it resulted in conductive polymers with a low band gap. We use specifically designed diketopyrrolopyrrole-based monomers for the on-surface Ullmann coupling reaction at the atomic scale and investigate the polymerization process using low-temperature scanning tunneling microscopy. After the formation of molecular wires on atomically clean Au(111) surface, their conductance is probed by STM lifting experiments. The obtained conductance value is among the best of all known molecular wires.



**Figure 1.** STM image of a fragment of a molecular wire grown on Au(111) substrate.

# Nano-electronic components built from DNA templates

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On the nanoscale, fundamental properties and potential applications are greatly influenced by the size and shape of the material. “DNA Origami” takes advantage of base complementarity of individual short oligonucleotides, to fold a long “scaffold strand” into almost any continuous 2D or 3D shape.<sup>[1]</sup> We recently introduced a new concept of DNA mold-based particle synthesis that allows the synthesis of inorganic nanoparticles with programmable shape. We demonstrated the concept by fabricating a 40 nm long rod-like gold nanostructure with a quadratic cross-section.<sup>[2]</sup> We expanded the capabilities of the mold-based particle synthesis to demonstrate the synthesis of uniform gold nanowires with controllable dimensions. Here the concept is further expanded by designing mold monomers with different geometries and interfaces, in which way, we can fabricate more complex ‘mold-superstructure’ in a unique and flexible way like lego bricks (see figure 1). We can also incorporate semi-conducting nano-rods into this mold-based system.

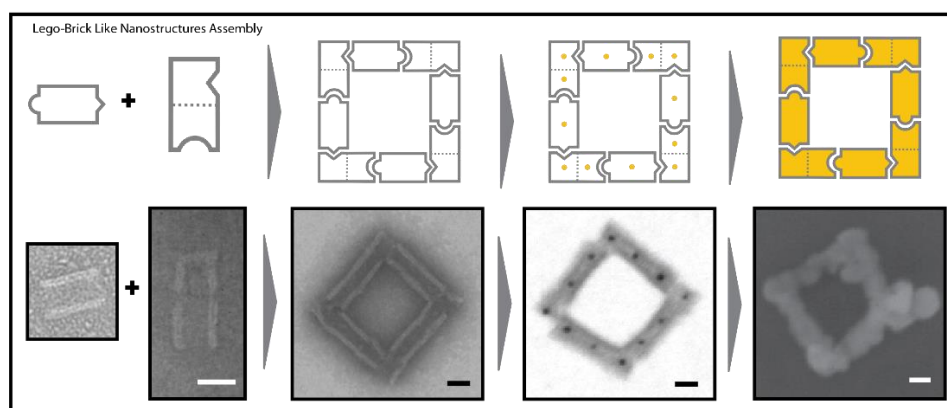


Figure 1. Sketch and TEM (SEM) images showing the Lego-Brick like nanostructure assembly of nano-circuit. By controlling the interface for the junction and mold structures, nano-circuit can form by just mixing the two monomers. With 5 nm gold seed decoration, the gold nano-circuit can be achieved with the same gold growth process. Scale bar: 20 nm.

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## Posters

updated: 14.08.2017 (PZ)

Presenter	No.	Title	Pg.
Awan	P1	Towards controlled modification of charge transport in two dimensional conductors	14
Baek	P2	Multiple Synaptic Modulation and Memory of Ionic Film-coated Si Nanowire Transistors for Neuromorphic Computing	15
Kilibarda	P3	Single Molecule Level Measurement: Study of Salen Molecule	16
Nikipar	P4	Theoretical methods for simulations of STM spectroscopy: the Tersoff-Hamann approximation and beyond	17
Perumallapelli	P5	2-Dimensional Hybrid Perovskites : Material and Electrical Characterizations	18
Schütt	P6	Dynamic impedance sensing of microorganisms using gold nanowires	19
Sekulla	P7	Polymer brush guided deposition of bio-macromolecule on solid surfaces	20
Sheng	P8	Template synthesis of 2D ultrathin polydopamine nanosheets	21
Skidin	P9	Asymmetry as a key factor for increasing the functionality of a molecular logic gate	22
Strobel	P10	Low temperature MCBJ measurements of C60 Fullerenes	23
Zhang	P11	Thermoresponsive on-chip microsupercapacitors	24

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2) Please, remove your poster latest on Friday noon.

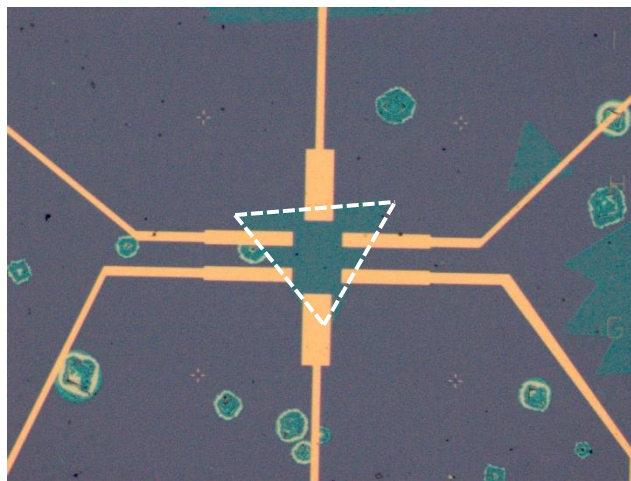
## Towards controlled modification of charge transport in two- dimensional conductors

Wajid Awan<sup>1</sup>, Antony George<sup>2</sup>, Andrey Turchanin<sup>2</sup>, Gregor Hlawacek<sup>1</sup>, Stefan Facsko<sup>1</sup>,  
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Layered transition metal dichalcogenides (TMDCs) which are two dimensional materials have drawn tremendous attention as promising channel materials with attractive electronic and optical properties for the next generation nanoelectronic devices. Despite the rapid progress in TMDCs device applications, the nature of charge transport still remains elusive. In particular, the physical properties of 2D thin nanosheets can be greatly affected and modified in controlled way by irradiation induced defects. Hence, it is important to have a good understanding of the effect of the ion irradiation on the properties of 2D thin nanosheets. In this work, we performed electrical transport measurements for CVD grown molybdenum disulfide ( $\text{MoS}_2$ ) and molybdenum diselenide ( $\text{MoSe}_2$ ) on  $\text{SiO}_2/\text{Si}$  substrate. Standard Electron beam lithography (EBL) was used to pattern the electrical contacts on flakes to fabricate the Field effect transistor (FETs) devices. For the purpose of sample characterization, Atomic force microscope (AFM) and Raman Spectroscopy techniques were performed to confirm the layer thickness which corresponds to a single layer. This knowledge was further used to controllably modify and tune the physical properties of thin 2D nanosheets by ion irradiation. We observe a change in conductance value by rastering the He ion beam of different fluences inducing the defects locally in the active channel area. Such defects introduce strong localized mid-gap states that act as scattering centers. Although these scattering centers do not open new transport channels, however they introduce a high anisotropy in the quantum conductance.



**Figure: Optical image of fabricated  $\text{MoS}_2$  FET device. The length scale is  $10\mu\text{m}$ .**



## Neuromorphic memory in multiplexed synaptic Si nanowire transistors with ion-doped film

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The brain has remarkable memory and learning ability using parallel information processing in multiple synapses. [1] By mimicking the brain functionality, artificial synapses have been established using memristors [2] and transistors [3] based on synaptic plasticity of ionic or memristive film. However, to realize the feasible memory and learning for neurocomputing is still in challenge because of the low compatibility with conventional Si-based CMOS process and unintuitive memory function using the timing between pre- and post-synaptic signals. [4] Here, we report synaptic Si nanowire transistors which have ion-doped silicate dielectric film. A planar top gate can simultaneously modulate the conductivity of many post-synaptic nanowires through the film, that would be able to realize multiple neurotransmission in the brain. The synaptic transistor acts as a random access memory (RAM) cell due to the movement of doped metal ions in the film depending on the amplitude and frequency of pulse on the gate. Therefore, the short term potentiation (STP) is configured by the transfer characteristics of the FETs. In addition, synaptic learning is shown after rehearsed training, so that the synapse quickly reaches the same current level before the training. This study has achieved a breakthrough in the convenient interconnection between neuromorphic device and CMOS system with tunable memory mimicking the process of human brain.

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[2] D. S. Jeong et al., RSC Adv. **3** (2013) 3169-3183

[3] H. Tian et al., Adv.Mat. **28** (2016) 4991-4997

[4] T. Serrano-Gotarredona et al., Front Neurosci. **7** (2013) 1-15

## Single molecule level measurements

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Current industrial scaling processes are reaching limits. We see not only diminished returns with further scaling attempts, but also physical limitations that come more and more into play.

In our research we offer a novel approach, where we try to drop altogether the concept of 3D scaling of electronic components and go to practically 1D molecular systems. This approach offers not only size improvements, but also reduction in power consumption and costs. Our research focuses on classifying different molecules with the help of Mechanically Controlled Break Junctions (MCBJ).

As a case study, we explore properties of salen molecule and its derivatives. Here we present the obtained results, namely, how chemical doping influences energy levels and affects electron transport through the molecule. Additionally, we present concepts for future devices which will allow us to explore thermal transport, as well as to explore the influence of gate potential on our systems.

## Theoretical methods for simulations of STM spectroscopy: Beyond the Tersoff-Hamann approximation

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We are working on the development of a theoretical platform to simulate the STM images and spectroscopy. The state-of-the-art atomistic simulations based on the density functional theory (DFT) and the Tersoff-Hamann approach for the tunneling current is usually applied to simulate the STM topography at small voltage. In addition, to capture the *spectroscopy results at finite voltage*, we employed the DFT based tight-binding model (DFTB approach) combined with the Green Function technique.

We developed the extension of the DFTB+ computational package for simulations of STM images and spectroscopy of molecules on metal surfaces. This approach offers a framework to calculate the tunneling current between tip and molecule more precisely, taking into account the tip geometry, it captures the interference and interaction effects, and simulate quantitatively the dI/dV map and spectroscopy curves. This new computational approach can be applied for the investigation of finite-voltage effects and describe the higher molecular transport states.

As an example, we consider diketopyrrolopyrrole (DPP)-based molecules on the Au(111) which were investigated experimentally. The calculated dI/dV maps of DPP monomers on Au(111) surface show good agreement with the experimental results.

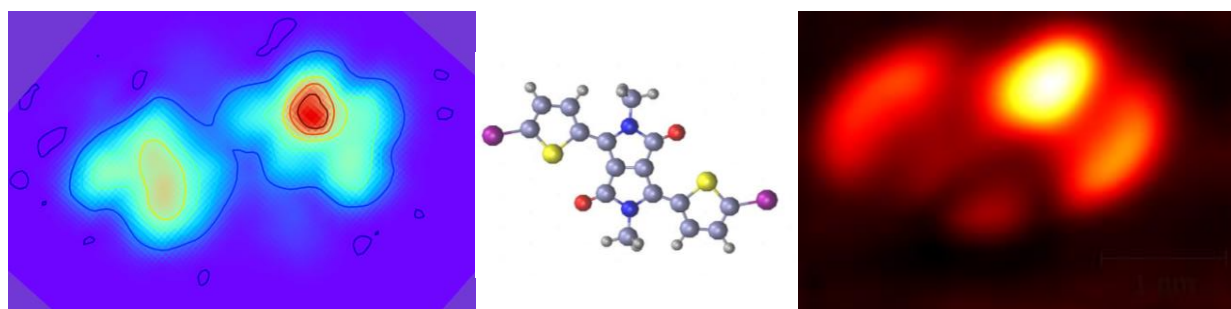


Figure: dI/dV map of the LUMO at 1V for a DPP monomer on Au(111) surface. Left: theoretical calculation. Right: the experimental result.

## 2D Hybrid Perovskites: Material and Electrical characterisation

Goutham Raj Perumallapelli<sup>1,2</sup>, Anton Kiriya<sup>1</sup> and Brigitte Voit<sup>1,2</sup>

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We report the material and electrical characterization of 4 different types of 2D hybrid perovskites which are mainly in the form of  $(R-NH_3)_2PbI_4$ , with different alkyl chains namely, Octyl, Butyl and Methyl amine to form,  $(Oct-NH_3)_2PbI_4$ ,  $(Oct-Me-NH_3)_2PbI_4$ ,  $(But-NH_3)_2PbI_4$  and  $(But-Me-NH_3)_2PbI_4$ . UV-Visible absorption spectroscopy has been carried out on the perovskite thin films and we have noticed that decrease in band gap ( $E_g$ ) is associated with a decrease in the alkyl chain in perovskite film.

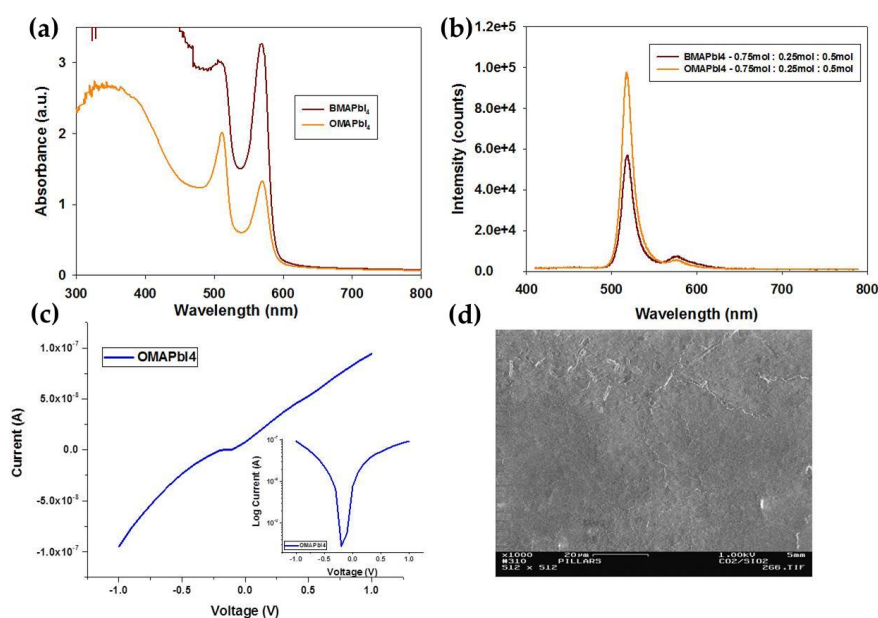


Figure1. (a), (b) are UV-Visible, Photoluminescence spectra of BMAPbI<sub>4</sub> and OMAPbI<sub>4</sub> perovskites respectively. (c) I-V characteristics of Octyl-methyl based perovskite thin film, inset: semi log scale IV characteristics (d) SEM micrographs of Octyl-methyl based 2D perovskite films.

Moreover, the absorption edges of octyl based perovskites are slightly red shifted from butyl-based perovskites. Similar behavior has been noticed in octyl-methyl and butyl-methyl based perovskites. Surprisingly, the 2D perovskite films are found to be mixture of multiple perovskite phases, with  $n = 1$  and  $2$ , where  $n$  is the number of semiconducting  $PbI_6$  octahedral units which is clearly evident from UV-Visible and PL spectra of perovskite thin films. Current-Voltage characteristics of perovskites exhibit a rectifying behavior indicating the formation of Schottky junction with electrodes, and they show the conductivity of  $1.05 \times 10^{-2}$ ,  $2.41 \times 10^{-2}$ ,  $3.80 \times 10^{-3}$  and  $1.70 \times 10^{-3} \text{ Scm}^{-1}$  for octyl, octyl-methyl, butyl and butyl-methyl based perovskites respectively. Unit cell dimensions of the perovskites have been extracted from X-ray diffraction spectroscopy. As expected, octyl-based perovskites have higher unit cell volumes than butyl based perovskites. Morphology of the perovskite films have been observed by using scanning electron microscope (SEM), and SEM images reveal the formation of flat and planar crystals. Both butyl and octyl based perovskites have crystal sizes varying from few hundreds of nanometers to several micrometers. Such morphologies seem to be beneficial for both the charge transportation and moisture protection.

# Nanoscaled impedance cytometry for bacteria analysis

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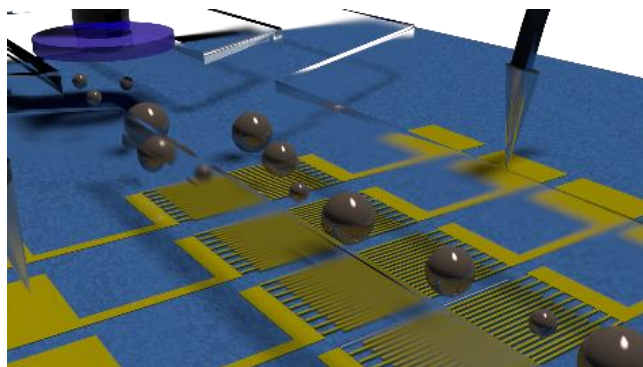
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Detection of pathogens at low concentrations and sample volumes is one of the mainstreams in the current biomedical research due to the distinct demographic changes and wide spreading of the chronic and severe illnesses. Conventional pathogen detection approaches enzyme-linked immunosorbent assay (ELISA), flow cytometry or DNA amplification using polymerase chain reaction require high effort and time with regard to sample preparation, signal processing and data analysis. Furthermore, since these techniques rely on optical detection, high sample volumes, analyte labeling and bulky equipment is mandatory.

Consequently, 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. In this, the next generation of bio-sensors for the detection of biological species also require high sensitivity and selectivity at high throughput due to low concentration of analytes, e.g. pathogens<sup>1</sup>, and in complex media like blood or saliva.

We faced the challenge to establish a MEMS-sensor capable of single bacteria detection based on dynamic impedance analysis. The detection of micron sized objects one by one is realized in flow, employing the cytometry principle (See Figure 1), converting the sample solution to interdigitating top-down fabricated gold nanowires<sup>2</sup>.



**Figure 1:** Schematic illustration of the nano-capacitor sensing device.

We demonstrate the detection of single particles in real-time based on impedance changes in a proof-of-principle approach as well as in-flow electrical differentiation of bacteria species.

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- [2] Takayanagi, K.; Kondo, Y.; Ohnishi, H.; JSAP Int. **3**, 3 (2001).

## Coating of DNA Origami with Polymer Brushes

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The interest in DNA origami has increased over the last decade. Their potential in nanoelectronics and photonics is one of the main focuses of researchers today. Still the lack of stability under salt and buffer free conditions hinders the application of DNA origami.

The first part of this thesis focuses on utilizing cationic poly(2-oxazoline)s (POx) for the coating and stabilization of DNA origami by forming polyplexes.

Those POx are polymerized *via* living cationic ring opening polymerization (LCROP). Due to a large variety of available 2-oxazoline monomers, those POx can be designed with numerous functionalities. By this, the overall functionalization of the origami can be increased.

The second part of this work focuses on depositing the produced polyplexes on sub- $\mu\text{m}$  patterned polymer brushes on solid surfaces. Investigation over the preferred orientation and the control over the orientation will be made, since this is of interest when it comes to the integration of DNA origami into electrical circuits.

# Polymer brushes on two-dimensional materials

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## Abstract

Two-dimensional (2D) materials have sparked increasing interest owing to their unique structures, wide range of chemical compositions, and a vast array of unique physical properties,<sup>[1-3]</sup> such as MoS<sub>2</sub>, MoSe<sub>2</sub>, WS<sub>2</sub>, WSe<sub>2</sub>, g-C<sub>3</sub>N<sub>4</sub>, black phosphorus. 2D materials have potential applications in electronic devices, optoelectronics, sensing, energy storage, and catalysis.<sup>[4-6]</sup> However, most of the above applications are still restricted to the structure of 2D materials in bulk, such as low dispersion and low-quality nanosheets, which results in low performance efficiency. Functionalization of such materials could facilitate the improvement of the surface properties of 2D materials, while also allowing for the tuning of their physical properties. Therefore, in this project, polymer brushes are used to modify the 2D materials and obtain functional the 2D materials (Figure 1, g-C<sub>3</sub>N<sub>4</sub> acts as a model system). We hope that this way can improve the optical, electronic and chemical properties of 2D materials.

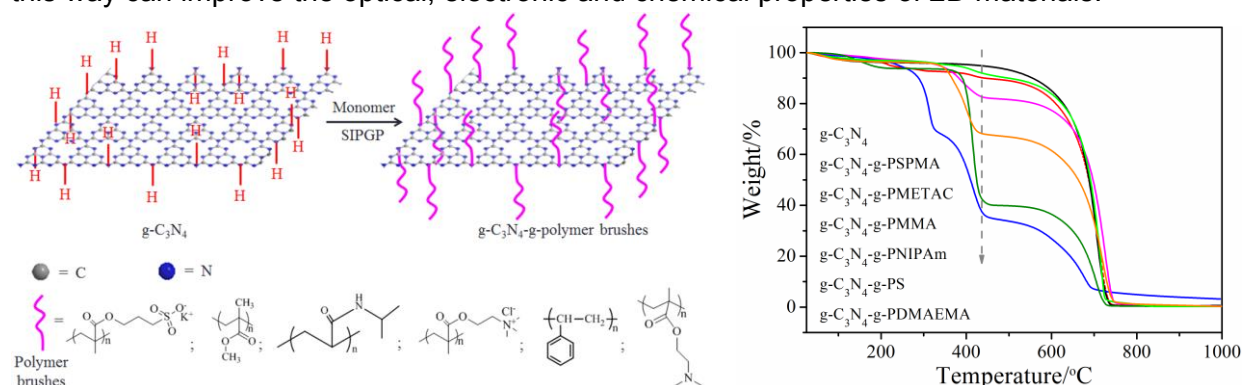


Figure1. Schematic illustration of preparing polymer brushes on g-C<sub>3</sub>N<sub>4</sub> particles and TGA curves of g-C<sub>3</sub>N<sub>4</sub> and modified g-C<sub>3</sub>N<sub>4</sub> (thermogravimetric analysis).

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## Asymmetry as a key factor for increasing the functionality of a molecular logic gate

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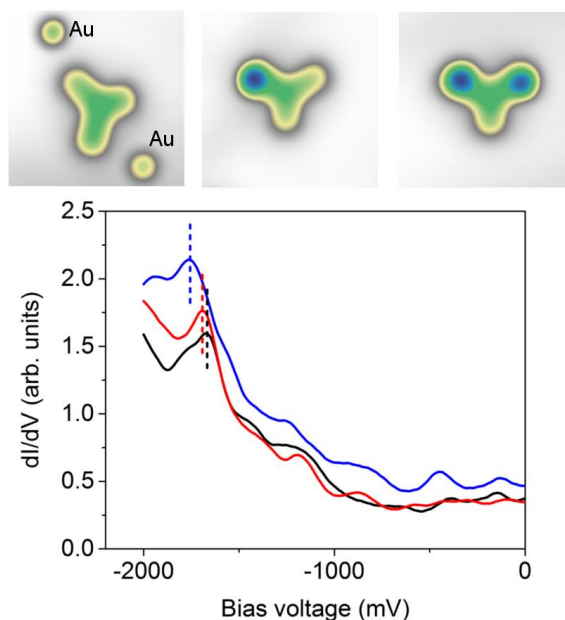
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Design and fabrication of nanoscale functional electronic units remains a main task of molecular electronics. Recently, it was shown, that by manipulating single gold atoms under symmetric starphene molecule, one could mimic the functionality of a NOR logic gate.<sup>1</sup> In our work, we investigate the role of asymmetry for the functionality of such a system. By applying classical gold inputs in different configurations, we can obtain various logical behavior of the system as an output, measured by the scanning tunneling spectroscopy. Thus, bringing the asymmetry into the molecule increases the functionality of a molecular logic gate. To fabricate a fully conjugated asymmetric starphene molecule on Au(111) surface, we employ surface-assisted cyclodehydrogenation.



**Figure 1.** Demonstration of NAND molecular logic gate by successively bringing Au atoms under the longer branches of an asymmetric starphene molecule.

Reference:

[1] Soe W.-H. et al., ACS Nano **5** (2) (2011) 1436-1440



# Low temperature MCBJ measurements of C<sub>60</sub> Fullerenes

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The poster shows the investigation of the conductance of C<sub>60</sub> Fullerene molecules using a unique mechanical controllable break junction (MCBJ) setup. The C<sub>60</sub> molecule with its high stability and symmetry is convenient to investigate the bonding between electrodes (Au) and molecule. The MCBJ setup enables to evaporate *in situ* and measure under high vacuum conditions. Furthermore, low temperatures measurements down to 10 K are compared with room temperature measurements. From conductance histograms preferred conductance values of single C<sub>60</sub> molecules are deduced. At room temperature more states appear for the same number of opening curves. At 10 K states are more stable; furthermore, the conductance state of a single C<sub>60</sub> molecule at 0.1 G<sub>0</sub> is clearly seen.

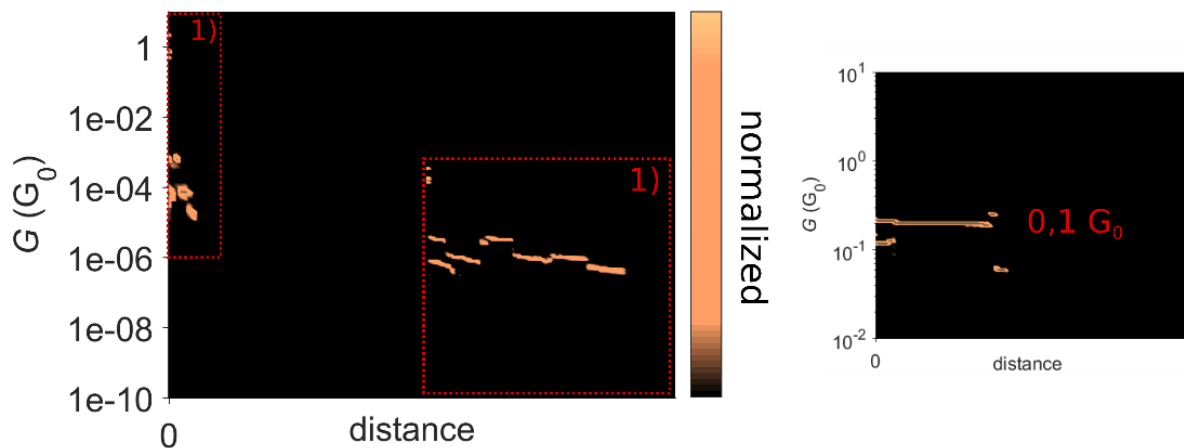


Figure 1: Conductance histogram of 15 opening curves at 10 K with the zoomed 0.1 G<sub>0</sub> state.

## Thermoresponsive on-chip microsupercapacitors

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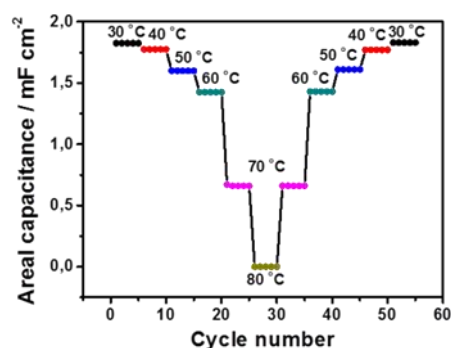
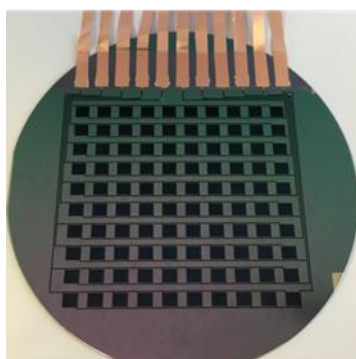
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On-chip microsupercapacitors (MSCs), as promising power candidates for micro-devices, typically exhibit high power density, large charge/discharge rates, and long cycling lifetimes. Unfortunately, as a result of rapid heat generation and accumulation in a limited space, severe thermal runaway in integrated micro-electronic devices including MSCs possibly leads to risks of fire or explosion. In this respect, thermoresponsive MSCs that feature a reversibly and sensitively temperature-dependent capacitive performance, is an appealing functional unit for realizing thermal protection toward miniaturized electronic devices. Here we design and fabricate a wafer-scale thermoresponsive MSC, which simultaneously functions as a micro-power storage device and thermal self-protection unit. Utilizing temperature-dependent thermodynamic behavior of a smart electrolyte (a lithium salt–dissolved polymer sol, poly(*N*-isopropylacrylamide)-*g*-methylcellulose), the ionic conductivity of the electrolyte greatly decreases and eventually switches off the MSC device at 80 °C and restores at room temperature upon cooling. In order to evaluate thermal-protection function of the MSC array, on-chip MSCs in series or parallel are fabricated. As the result, thermal protection toward the integrated devices is successfully realized using a single thermoresponsive MSC. Therefore, thermoresponsive MSCs are promising component in the thermal protection of practical on-chip electronic devices.



## **Your Notes**

## **Your Notes**

## **Your Notes**

## Hiking Tour to the Klingenberg Dam (3.9km, 1:09h)

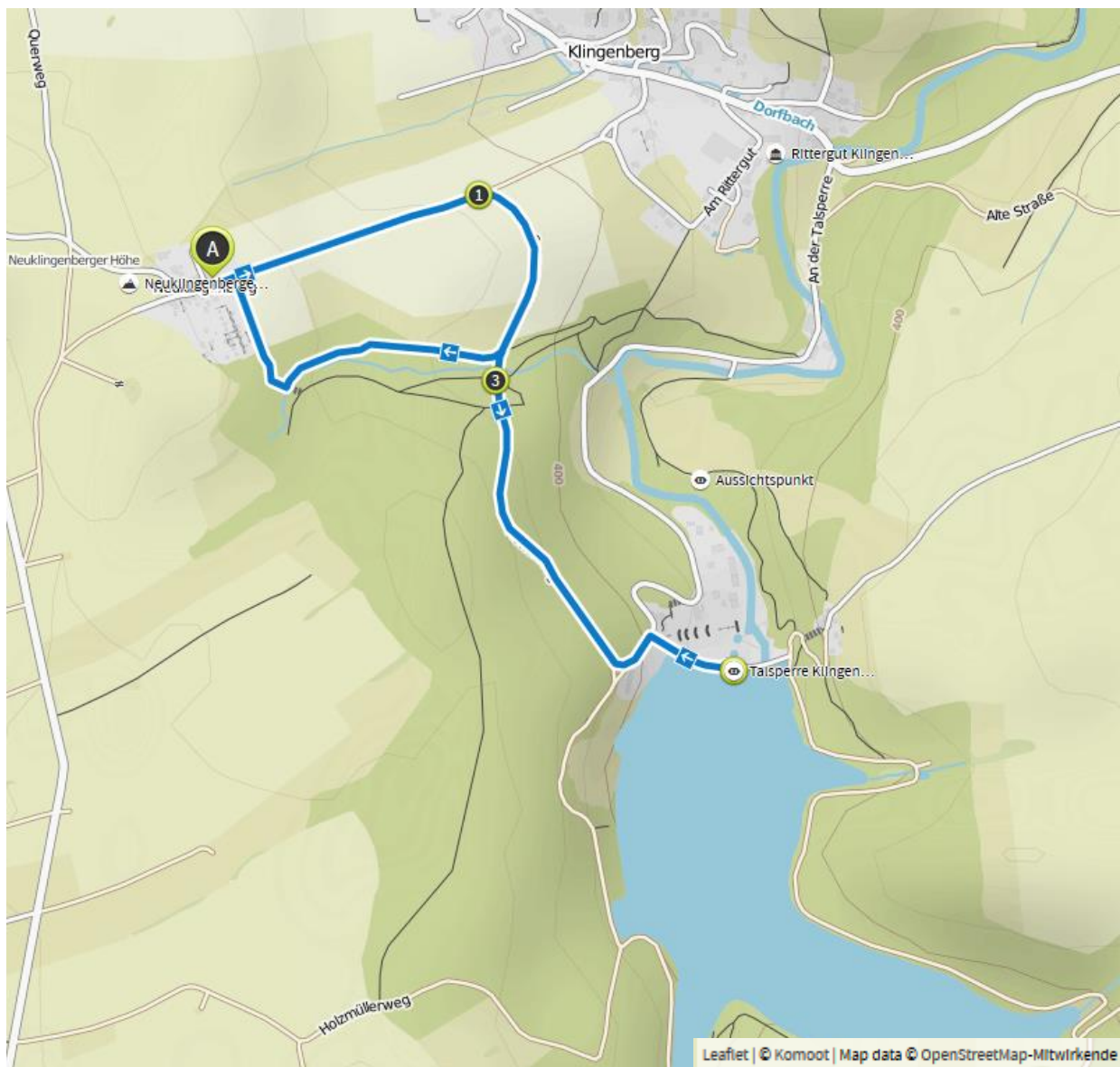
### A: Hotel Neue Höhe

#### 1: turn to the right

#### 2: View from the top of the Dam (Talsperre Klingenberg)

The dam was erected between 1908 and 1914. It provides the drinking water for the Dresden area to a large extent.

**3: Streichholzbrücke – Fire match Bridge** built between 1910–1911 as wooden railway bridge, changed to a Road Bridge in similar form in 1924, today a technical monument.



## NanoNet Annual Workshop 2017, Klingenberg

### Participants

Updated: 14.08.2017 (PZ)

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