

International Helmholtz Research School  
for Nanoelectronic Networks

# IHRS NANO NET Annual Workshop 2018

5 – 7 September 2018

Berghotel Augustusberg, Bad Gottleuba, Germany



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## Venue and organization

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## Agenda

Place: Hotel Augustusberg, Augustusberg 15, 01816 Bad Gottleuba  
updated: 03.09.2018 (PZ)

### Wednesday, 5 September 2018

Start	Who	Durat.	Title	Notes
10:00			Shuttle transfer from station <b>Dresden Hbf</b>	
12:00			Arrival/Lunch Buffet	
13:30	Erbe, A.	10	Welcome address	Chair: Zahn
13:40	Stampfer, C.	40+10	Extraordinary high room-temperature mobility in graphene-WSe <sub>2</sub> heterostructures	
14:30	Davitt, F.	25+5	2-D to 1-D Growth of Layered SnSe <sub>2</sub> : Morphological Control of CVD Grown Nanostructures	
15:00		30	Break	
15:30		90	<b>Poster session</b>	12 Posters
17:00			<b>Walking Tour – Gottleuba Valley View</b>	
19:00			Dinner	

### Thursday, 6 September 2018

9:00	Metzger, R.	40+10	Quo Vadis, Unimolecular Electronics?	Chair: Joachim
9:50	Nikipar, S.	25+5	STM images and spectroscopy of molecules on metal surfaces: DFTB+XT computational platform	
10:20		30	Break	
10:50	Jordan, R.	40+10	From Self-assembled Monolayers to Polymer Brushes (2)	Chair: Seidel
11:40	Günther, F.	25+5	A Novel Hybrid Material for Stretchable Semiconductor Applications	
12:15			Lunch	
13:45	Kelling, J.	25+5	Data Analysis and Machine Learning at the Computational Science Group	Chair: Gemming
14:15	Schütt, J.	25+5	Integrated nanoscaled biodetectors of biochemical species	
14:50		30	Break	
15:30			<b>Sightseeing Marie-Louise-Stolln</b> (Bus Departure)	
19:00			BBQ Dinner	

### Friday, 7 September 2018

9:00	Joachim, C.	40+10	Single molecule logic gates	Chair: Lissel
9:50	Baek, E.	25+5	Tunable memory and learning of Si nanowire transistors using history-dependent pseudo gate for physical neural network	
10:20		30	Break	
10:50	Zahn/Erbe	40	Annual Meeting: Status & Future, NanoNet Conference 2019	Chair: Erbe
11:30	Arora, H.	25+5	Effective passivation of air-sensitive two-dimensional materials to enhance their electrical properties	
12:15			Lunch incl. Student Award Ceremony	
14:00			Departure (Shuttle bus to Dresden Hauptbahnhof)	

Breakfast will be served from 7 a.m.

## NanoNet Annual Workshop 2018, Augustusberg

### Talks

updated: 03.09.2018 (PZ)

Presenter	No.	Title	Pg.
<b>Invited Talks</b>			
Joachim, C.		Single molecule logic gates	3
Jordan, R.		From Self-assembled Monolayers to Polymer Brushes- Part II: Polymer Brushes	4
Metzger, R.M.		Quo Vadis, Unimolecular Electronics?	5
Stampfer, C.		Extraordinary high room-temperature mobility in graphene-WSe <sub>2</sub> heterostructures	6
<b>Contributed Talks</b>			
Arora, H.		Effective passivation of air-sensitive two-dimensional materials to enhance their electrical properties	7
Baek, E.		Tunable memory and learning of Si nanowire transistors using history-dependent pseudo gate for neurocomputing	8
Davitt, F.		2-D to 1-D Growth of Layered SnSe <sub>2</sub> : Morphological Control of CVD Grown Nanostructures	9
Günther, F.		A Novel Hybrid Material for Stretchable Semiconductor Applications	10
Kelling, J.		Data Analysis and Machine Learning at the Computational Science Group	11
Nikipar, S.		STM images and spectroscopy of molecules on metal surfaces: DFTB+XT computational platform	12
Schütt, J.		Integrated nanoscaled biodetectors of biochemical species	13

List of Poster Contributions see page 16.

# Single molecule logic gates

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## Abstract:

The architecture of a molecule(s) Boolean logic gate can be classical, semi-classical or quantum [1]. Classical is supposing the interconnection of elementary active devices like molecule-switches or molecule-rectifiers with molecule-transistors using conductive nanowires to form the logic gate circuit [1]. Such an hybrid molecular circuit can appriori lead to a complex Boolean logic function if power gain exists per logic layer [2]. Semi-classical is based on the chemical bonding of molecular wires and active molecular devices together to form a single and large molecule-circuit where the total electronic circuit is embedded in one molecule [3]. Some logic gates have been recently designed this way but using intramolecular circuit rules different from the G. Kirchhoff circuit rules. The first verification of those intramolecular circuit rules was recently performed on a single molecule [4, 5].

Going quantum, the orthodox quantum computing approach is based on the control of the spontaneous response in time of a molecular quantum system structured in weak interacting qubits to perform certain tasks [6]. The logical inputs are encoded in this initial quantum state of the input qubits register and the quantum system evolves in time. The specific states reached during this time evolution is carrying the logical output. A few qubits molecules have already been proposed for single molecule experiments on a surface [6,7]. With our new Quantum Hamiltonian Computing (QHC), the complex functionality of a Boolean logic gate is implemented inside one molecule by inputting the logical information on its chemical skeleton and by measuring the logical output using the Heisenberg-Rabi oscillation frequency when oscillating between always the same initial and final quantum states per outputs [8]. Contrary to the Feynman-Deutsch quantum computing approach [6], those initial and final states are carrying no direct information on the implemented logic function. QHC has the advantage to required no structuration of the molecule in qubits and to avoid the problem of the current intensity exponential decay of the semi-classical approach [4]. Without embedding rectifiers, switches, transistors or qubits along the molecule, a QHC molecule can compute in a quantum way. Following this approach, a first QHC NOR molecule gate have been experimentally demonstrated [9], an XOR gate and recently a molecule  $\frac{1}{2}$  adder designed with 4 graphene nano-interconnects [10].

## References

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# - From Self-assembled Monolayers to Polymer Brushes - Part II: Polymer Brushes

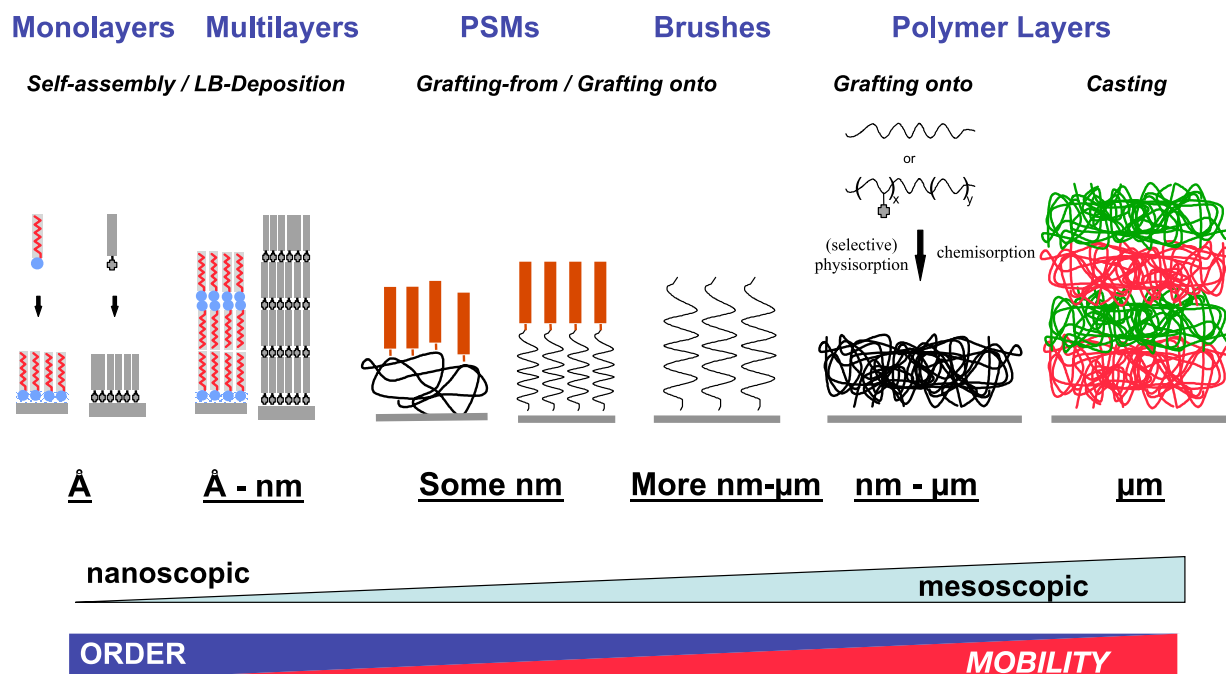
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This tutorial lecture series give a brief overview on the preparation and properties of self-assembled monolayers (SAMs) (Part I) and their use as two-dimensional initiator systems for the preparation of polymer brushes by means of surface-initiated 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" and recent results of the preparation of hydrophobic polymer brushes in water.



## Quo Vadis, Unimolecular Electronics?

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Unimolecular Electronics (**UME**) began with (i) the seminal paper by Ari Aviram and Mark Ratner [1], (ii) an inspiring talk “There is Plenty of Room at the Bottom” by Richard P. Feynman [2], (iii) the increases in device speeds in commercial inorganic integrated circuits as the device dimensions were halved every 18 to 24 months [3].

The first organic rectifier was measured in England [4] and verified in Alabama [5]. It is fair to say that the field of Unimolecular Electronics has progressed and matured [6].

The UME idea was simple and appealing: single molecules, designed to have “electroactive properties” as one-electron donors D or as one-electron acceptors A (or appropriate combinations of D and A [2]), when properly configured in space (i.e. contacted by appropriate electrodes) and measured at the “right” voltage to bring the molecular properties into resonance with the metal electrodes, would be a nanoscopic replacement for inorganic Si-based or Ge-based microscopic p-n or n-p rectifiers or even n-p-n transistors. Where are we? Where are you going, UME [6]?

- (A) The race to the bottom, e.g. to 10 nm device half-pitch, was won by the semiconductor industry (Intel, Samsung, etc.) with no help from organic chemistry.
- (B) However, molecules in excited states can easily decay by photon emission, not phonon emission, and thus avoid circuit over-heating.
- (C) A recent monolayer rectifier has achieved an impressive rectification ratio  $RR \equiv -I(V) / I(-V)$  of 165,000 [7].
- (D) A transistor molecule has been proposed [8] but not tested.
- (E) The interplay between molecular energy levels at resonance with metal electrodes is much better understood.
- (F) The electrode design needs more attention.

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# Extraordinary high room-temperature mobility in graphene-WSe<sub>2</sub> heterostructures

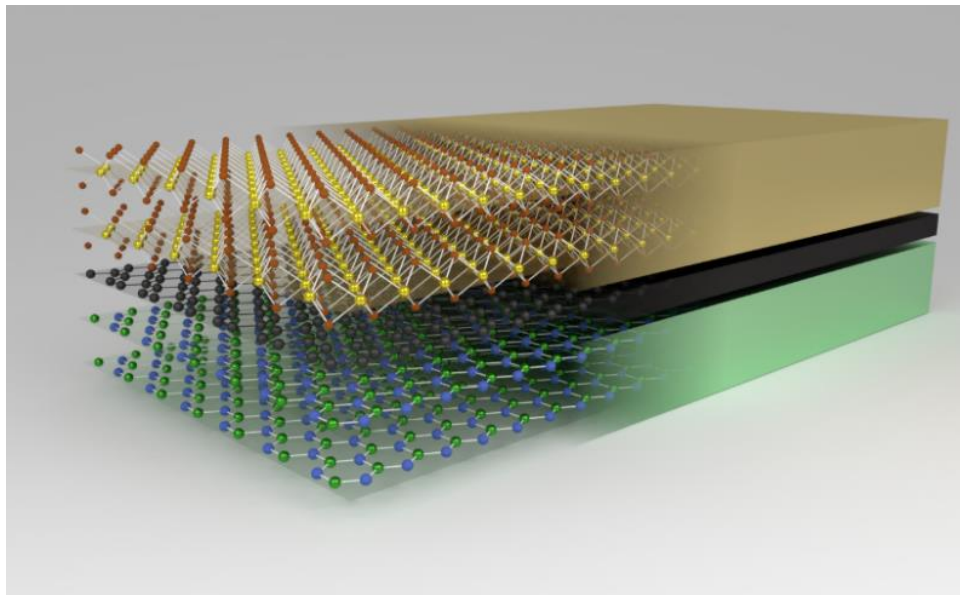
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Over the past years many promising applications of graphene have been demonstrated on individual devices. In order to advance from basic research towards scalable industrial applications, large area high quality graphene is needed. One promising approach to achieve this is chemical vapor deposition (CVD) of graphene on copper. However, so far the charge carrier mobility of CVD grown graphene has been significantly lower than what has been observed in devices fabricated from exfoliated graphene. Here, I will show that the electronic quality of CVD graphene depends critically on the transfer method and we present a novel dry transfer technique for CVD-grown graphene crystals that yields devices encapsulated in hexagonal boron nitride (hBN) with carrier mobilities up to 850,000 cm<sup>2</sup>/(Vs). In addition to the diffusive transport in such samples, we demonstrate an elastic mean free path exceeding one micrometer at temperatures of up to 200 K using Hall cross devices. By investigating large samples we furthermore conclude that the mean free path can exceed 25 micrometer at 2 K. I will discuss strategies for reaching the intrinsic electron-phonon limited carrier mobility in CVD graphene showing that the electronic properties of CVD-grown "synthetic" graphene can in principle match those of ultrahigh-mobility exfoliated "natural" graphene. Finally, I will show that the graphene-WSe<sub>2</sub> heterostructures (see Figure) allow for ultra-high mobility devices exceeding state-of-the-art devices based on hBN-graphene-hBN.



**Figure:** Illustration of a 2D heterostructure consisting of 2 layers of hexagonal boron nitride (bottom), graphene and 2 layers of WSe<sub>2</sub>.



# Effective passivation of ultra-thin layers of InSe to enhance electrical properties

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Here, we report electrical properties of ultrathin layers of Indium Selenide (InSe), a member of the III-VI chalcogenides family, which has shown a mobility two orders of magnitude higher than MoS<sub>2</sub>, alongside better stability than black phosphorus.

InSe has light electron effective mass ( $m^*=0.143 m_0$ ) and high mobility ( $10^3 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$  at room temperature) enabling its usage for fast, high performance electronics. State-of-the-art InSe field-effect transistors reported so far, consist of 8 nm thick InSe flake contacted using graphene edge contacts to form source and drain. The device reached a mobility of  $1270 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$  at room temperature in top-gate configuration <sup>[1]</sup>. However, InSe being an air-sensitive material loses its conductance over time, resulting the transistor becoming unfunctional <sup>[2]</sup>.

In this study, we report an InSe-based transistor fully encapsulated in h-BN layers which enhanced its electrical properties compared to an un-encapsulated device. The transistor showed a high mobility at room temperature, while retaining its performance over a long period of time. The full encapsulation of InSe flakes gave us an opportunity to understand its transport mechanisms in much greater details.

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# Tunable memory and learning of Si nanowire transistors using history-dependent pseudo gate for physical neural network

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Today's physical neural network system is built using non-volatile memristive devices with digital input signaling. In reality, the brain and neurons represent a dynamic system, which performs oscillation and synchronization for information processing and communication based on short-term (working) memory in the analog regime. Therefore, emulating the dynamic property of the neuron is significant to build a real brain-like computing machine.

Here, we demonstrate *tunable memory* of a Si nanowire field-effect transistor which is modulated by sol-gel derived pseudo gate layer. The sol-gel derived layer is doped by metal ions which are mobile once bias voltage is applied. Thus, the intrinsic material property, such as drying condition and ion concentration of the film, is able to tune the memory capability of the device. As a result, the device acts as a dynamic volatile memory with long retention time. Also, the ionic polarization of the pseudo gate layer allows the device to emulate neuronal membrane functionality. The ionic states within the sol-gel film store the history of input signals, thereby enabling the learning capability of the device. Therefore, the device can eventually merge the memory and learning functionality in one transistor device like a neuron, which would be a key computing element of the physical neural network.

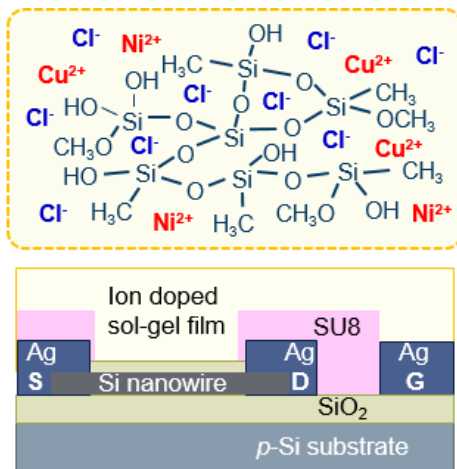


Fig. 2: Chemical structure of the film and the device structure

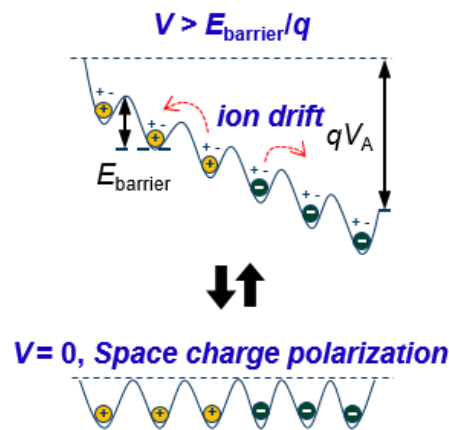


Fig. 1: Ionic dynamics in the film with applied bias

## 2-D to 1-D Growth of Layered SnSe<sub>2</sub>: Morphological Control of CVD Grown Nanostructures

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Bottom-up growth strategies offer the potential for precise control over the crystallinity, structure, composition, and morphology of nanomaterials. In this research, a liquid injection chemical vapor deposition method has been utilized to grow crystalline tin diselenide (SnSe<sub>2</sub>) nanostructures, from a distorted octahedral [SnCl<sub>4</sub>{<sup>n</sup>BuSe(CH<sub>2</sub>)<sub>3</sub>Se<sup>n</sup>Bu}] single source diselenoether precursor.<sup>1</sup> Most notably, careful adjustment of the growth parameters yielded great morphological control of the grown nanostructures; yielding structures from large 2D flakes, to large branched wire networks, and individual one-dimensional (1-D) nanostructures. With the custom designed single source precursor, SnSe<sub>2</sub> nanostructures of only a few layers thickness were achievable, as well as 1-D growth with diameters between 60-240nm.

The Sn:Se stoichiometric ratio of ~1:2 in all of the different morphologies was confirmed by energy dispersive X-ray analysis and Raman spectroscopy. The presence of the SnSe<sub>2</sub> A<sub>1g</sub> Raman mode was clearly observed for all synthesized nanostructures.<sup>2</sup> The morphology and crystal structure of the SnSe<sub>2</sub> nanostructures was investigated through X-ray diffraction, atomic force microscopy, electron diffraction, and transmission electron microscopy.

SnSe<sub>2</sub> nanostructures demonstrate potential applications in phase change memory devices (PRAM), with films of SnSe<sub>2</sub> being previously reported as showing the reversible amorphous to crystalline switching needed in phase change memory applications.<sup>3,4</sup>

### References

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<sup>2</sup> Smith, a. J et. al. *J. Phys. C: Solid State Phys.* 10 (1977), 1321.

<sup>3</sup> Chung, K.-M. et. al. *J. Appl. Phys.* 103 (2008), 83523.

<sup>4</sup> Wang, R. Y. et. al. *J. Appl. Phys.* 109 (2011), 113506.

## A Novel Hybrid Material for Stretchable Semiconductor Applications

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To make the visions that we have for our future to become true, especially to fulfil the expectations for the electronic devices, new materials are needed. In the past decades, organic materials have been intensively studied since they show some advantages over bulk semiconductors. For instance, they offer the possibility to fabricate flexible devices. So far, flexibility has mainly been studied in terms of bendable or twistable devices. Hence, the next stage on the road map towards higher functionality is to focus on stretchability.

In this presentation, a novel hybrid material is suggested which is based on diketopyrrolopyrrole (DPP) and poly(dimethylsiloxane)urethane (PDMSUr). The former is the currently leading compound of semiconducting polymers, whereas the latter is a rubber material, which offers a huge playground to vary the mechanical properties by controlling chain lengths and cross-linking. We will give an overview on the state-of-the-art of stretchable materials and introduce a research plan how we intend to synthesize and characterize this novel material.

# Data Analysis and Machine Learning at the Computational Science Group

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In this talk I will summarize the current activities of the computational science group at HZDR, which range from establishing research data publication (RODARE) and management platforms to providing numerical and computational expertise in various research projects. The latter aspect will be presented in detail through two selected ongoing projects.

In a project with the institute for resource ecology at HZDR, we developed a framework for the analysis of spectra of mixed solutions. The goal of the analysis is to discover how many species are in a given sample and in what concentration while at the same time extracting their unknown spectrum. A number of numerical techniques can be employed to this end, each requiring different amounts prior knowledge and different types of measurements. Here the primary task of the analysis framework is to unify a zoo of different implementations of similar methods and making all methods available to all scientists. Additionally, it enables simple use of remote computing resources, which allow for more computationally intensive analysis which can add a more reliable way to estimate confidence bounds.

In another project, we are using deep learning approaches to develop an automated safety system for the high-power laser systems DRACO and PENELOPE at HZDR. Here the goal is to detect defects or scatterers which focus parts of a yet unfocussed beam. These can, when left unchecked, cause cascades of failing mirrors, lenses, and non-linear crystals and should thus be detected in the time between two shots. This work uses deep convolutional neural networks implemented through the Caffe framework to achieve real-time detection and localization of impurities in the beam profile.

# Simulation of STM images and spectroscopy of molecules on metal surfaces: DFTB+ computational platform

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In this work, we developed a theoretical and computational approach for simulations of STM images and spectroscopy, in particular of molecules on metal surfaces. We employed the DFT based atomistic tight-binding model (DFTB approach) combined with the Green function technique, which offers a framework to consider a tip, molecule and surface as one integrated system and taking into account the tip geometry. Besides, it captures the interference and interaction effects. This new computational approach can be applied for the investigation of finite-voltage effects and describe the higher molecular transport states. It allows to calculate the tunneling current between a tip and a molecule more precisely, and simulate quantitatively  $dI/dV$  maps and spectroscopy curves. We developed the extension of the DFTB+ computational package ([dftbplus.org](http://dftbplus.org)), which makes possible and convenient calculations for large-scale molecular nanosystems on metal surfaces. Our approach is quite fast due to the DFTB approximation and the effective MPI parallelization. The DFTB+ is free software and can be used at HPC clusters.

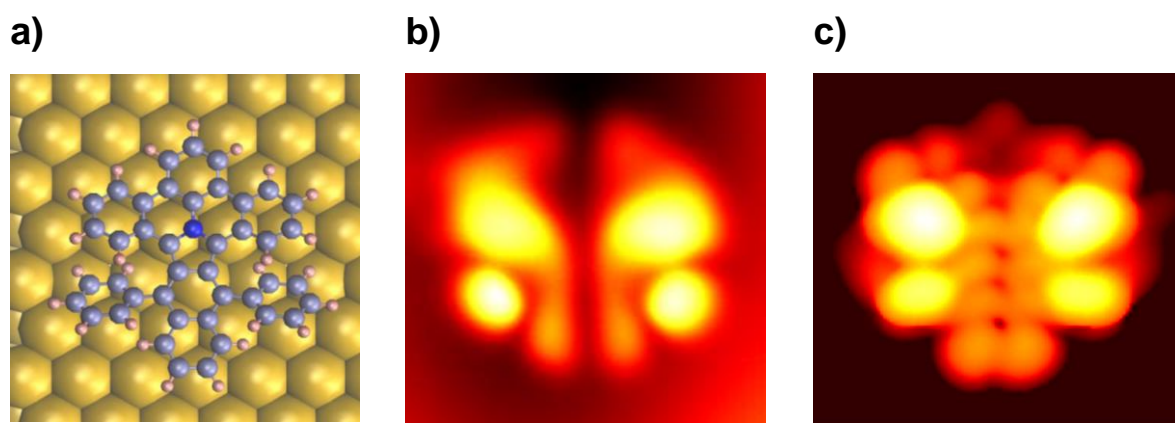


Figure: a) Relaxed Azaacene 5, 7 molecule on Au(111) surface; b) experimental results for  $dI/dV$  map (HOMO) at -0.38 V ; c) theoretical simulation  $dI/dV$  map (HOMO) at constant current mode, all three images are in same scale and size.

# Integrated nanoscaled biodetectors of biochemical species

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Worldwide demographic changes and high distances to clinical institutions, especially in rural regions, demand a new generation of disease diagnostic sensors offering high transportability, small scale and easy handling at low costs. Here, conventional methods for disease detection are restricted to laboratory institutions and require trained personnel with costly operation and long analysis times. The development of “lab-on-a-chip” biosensors enables the transfer of state-of-the-art detection methods onto small chip scale allowing a simpler and cheaper detection, even applicable for untrained personnel. In contrast to conventional methods, which mostly rely on optical detection and its analysis, „lab-on-a-chip“ biosensors are capable of detecting biospecies electronically by introduction of electronic detection blocks like field effect transistors and capacitors. Additionally, introduction of nanoscaled geometries drastically improves the sensitivity of these devices.

This work demonstrates the development and integration of two electronic detection elements in microfluidic structures as well as their suitability as biosensors. The first part of this work is dedicated to the integration of emulsion-based microfluidics on silicon nanowire field effect transistors and the label-free detection of microfluidic droplets based on their chemical composition. The second part deals with the development of a sensor platform, reconstructing the methodology of „flow cytometry“ on chip scale. Instead of optical detection, this chip utilizes gold nanowire capacitors as electrochemical detection mechanism, recording impedance alterations in presence of biospecies.



## **Your Notes**

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## NanoNet Annual Workshop 2018, Augustusberg

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updated: 31.08.2018 (PZ)

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

# 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 nano-electronics and nano-photonics device fabrications. This technique enables the precise positioning of metallic and semiconducting nanoparticles along the DNA nanostructures. In this study, DNA origami nanomolds<sup>1,2</sup> and nanosheets are used for the fabrication of nano-electronic devices. To this end, electroless gold deposition is used to grow the AuNPs within the DNA origami nanomolds and nanosheets create eventually continues nanowires. In order to contact the fabricated nanostructures electrically, a method using electron-beam lithography was developed. The DNA origami nanomold and nanosheet based metallic wires were electrically characterized from room temperature down to 4.2K.

Temperature-dependent characterizations for four wires exhibiting different conductance at RT were performed in order to understand the dominant conductance mechanisms from RT to 4.2K. Two of these nanowires based on nanomold structure showed metallic conductance.<sup>1</sup> The other wires deviated from pure metallic behavior and they showed thermionic, hopping and tunneling charge transport mechanism.

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# Semiconducting Organosilicon-based Hybrids for the Next Generation of Stretchable Electronics

Kristina Ditte<sup>1</sup>, Dr. Franziska Lissel<sup>1</sup>, Dr. Anton Kiriya<sup>1</sup>, Prof. Brigitte Voit<sup>1</sup>

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The future world is expected to be full of smart electronics and communication devices integrated in clothes, tools and even interacting with the human body. This requires new materials which are electronically active and mechanically soft and stretchable. Polymer semiconductors (PSCs) are promising as they are soft in comparison with inorganic materials and allow the fabrication of thin film devices.

Yet state-of-the-art PSCs are brittle and prone to mechanical failure<sup>1</sup>, preventing roll-to-roll manufacturing<sup>2</sup>, the integration into clothing or the utilization in strenuous environments. The goal of my Ph.D. project is to develop intrinsically flexible and stretchable PSCs by combining the excellent electronic properties of state-of-the-art diketopyrrolopyrrole (DPP) based donor-acceptor (D-A) block copolymers<sup>3</sup> with the favorable mechanical properties of polydimethylsiloxane (PDMS) elastomers<sup>4</sup>. This will be achieved by creating “second order” block copolymers (Fig. 1), i.e. by alternating rigid-rod PSC units and short PDMS chains. Utilizing components of a defined length and combining them in a controlled fashion allows to preserve their inherent mechanical and electronic properties. In the resulting well-defined second-order hybrid, the two components are expected to compartmentalize into separate stacks, thereby ensuring lateral charge transport through the D-A stacks well-separated by elastic PDMS “springs”, which are in turn responsible for overall material elasticity. In later stages of the project, the mechanical properties of the “second order” copolymers will be tuned, e.g. by changing the lengths of the PDMS unit or by crosslinking these units<sup>4</sup>. Also the utilization of PDMS sidechains for regular high-performance D-A block copolymers will be explored.

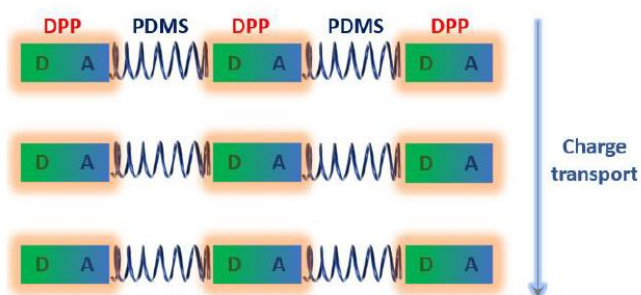


Figure 1. Schematic representation of a stacked “second order” block copolymer comprised of D-A units and short PDMS chains.

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## P-doped Ge nanowires fabricated by electron beam lithography

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Germanium (Ge) is a promising high mobility channel material for future nanoelectronic devices, which is a Carbon group (IV) semiconductor with a lower effective charge mass than Silicon (Si), resulting in a higher electron ( $\times 2$ ) and hole ( $\times 4$ ) mobility. Materials with high carrier mobility can enable increased integrated circuit functionality or reduced power consumption. Hence, Ge based nanoelectronic devices could offer improved performance at reduced power consumption compared to Si electronics. Doping or introduction of impurity atoms allows tuning of the electrical properties of the semiconductor material, which is related to access resistance. Ion beam implantation is an industrial standard for semiconductor's doping as it can generate a single ion species with a single energy in an industrially friendly highly controlled fashion. The destructive nature of ion implantation doping due to the deposited energy and resultant cascade recoils within the nanowire volume requires a crystal recovery step such as an annealing process. In this work, Ge nanowires were fabricated using electron beam lithography (EBL) and ion beam implantation was used to introduce Phosphorous (P) dopant atoms in Ge Nanowires. Then, due to destructive nature of ion beam implantation method, flash lamp annealing (FLA) was applied to recover the crystal structure of Ge nanowires and activate the dopant atoms. The electrical properties of doped nanowires were measured using four-probe configurations. Moreover, micro-Raman spectroscopy was utilized to investigate the impurity and crystallite characterizations of the substrates.

## **High-quality Seedless Group IV nanowires: Synthesis and Characterization**

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The recent years have seen an explosive interest in one-dimensional nanostructures and germanium is positioned as the mainstream material for nanoelectronic applications. Bottom-up growth of Germanium nanowires usually involves metal-seed (Au most popular) nanoparticles as catalyst in a three phase vapor-liquid-solid (VLS) like growth paradigm. The use of non-contaminating metal catalysts (or self-catalytic) facilitate the direct integration of nanowire components into future devices.

Broad number of experiments have been screened to fully understand the role that toluene and long carbon chains (or other similar organic compounds) can play on the growth of the group IV wires. Closed-cell set-up has been chosen as an alternative of the classical CVD approach for seedless nanowire growth because it utilizes a simplified process where reaction takes place under high pressure (toluene in Supercritical Fluid phase).

In-depth study (HRTEM, FTIR, XPS etc.) on the high-quality Ge NWs, Sn NWs and GeSiSn NWs has been carried out for a better understanding of growth mechanism and structural and physical properties.



# Controlled Nickel Silicidation using Flash Lamp Annealing for Reconfigurable Field Effect Transistors

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Reconfigurable field effect transistors (RFET) can be tuned to *p-or n-* polarity by applying appropriate electrostatic potential at gate. Therefore, functional complexity and performance of electronic circuits can be enhanced using such FETs. To fabricate an RFET Silicon (Si) nanowires (NWs) are silicided at both ends to form Si-NiSi<sub>2</sub>-Si Schottky junctions. Formation of NiSi<sub>2</sub> is a pre-requisite for proper operation of these devices because metal work function of NiSi<sub>2</sub> aligns itself near the mid-bandgap of Si, thereby enabling band bending by application of electrostatic potential for its function as *p/n* FET. Previous studies have shown formation of NiSi<sub>2</sub> by rapid thermal annealing (RTA) but proper control over silicide length has not been achieved which limits the prospect of Si channel scaling.

We report on SiNWs silicidation performed using flash lamp annealing (FLA). The SiNWs are fabricated on silicon on insulator (SOI) substrates by a top down process based on electron beam lithography (EBL) and subsequent inductively couple (ICP) etching. Thereafter, nickel(Ni) is evaporated at lithographically defined areas. Finally FLA is performed, which yield Ni silicide-Si Schottky junctions. FLA based silicidation process provides better control over the progression length of silicidation along the SiNWs compared to RTA based process.

This FLA process is optimized by performing annealing with different values of time and flash power by adjusting these values such that the resulting temperature remains same in all cases. Moreover, FLA was done in different gas environments to study their effect on resulting electrical characteristics. The difference of silicide length is much smaller in FLA samples as compared to RTA ones. Therefore, this process allows much better control on Schottky junction positioning and, hence, enables Si channel scaling. The results of SiNW silicidation in different crystal orientations NWs will be presented at conference.

## Single molecule electron transport characterization

Filip Kilibarda<sup>1</sup>, Alexander Strobel<sup>1</sup>, Torsten Sendler<sup>1</sup>, Michael Mortensen<sup>2</sup>, Kurt Gothelf<sup>2</sup>, Artur Erbe<sup>1</sup>

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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 Junction (MCBJ).

Here we present measurements on two different systems. The one of them is salen complex. We try to explore the influence of different ion inclusions on electron transport through the molecule and how “chemical doping” changes the energy levels. Additionally, we can observe effect of the spatial structure on stability of the junction.

The other molecule of interest is corannulene. It consist of bowl shaped center, which represents segment of the c60 molecule. It offers good transport properties due to many conjugated bonds. Abundance of conjugated carbon bonds and spatial structure of the molecule offer a good building block for future attempts at gating and inclusion of donor/acceptor groups.

## **Investigations of PEEB adsorbed on Au(111) surfaces**

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The electronic and tunable optical properties exhibited by p-phenylene-ethynylenes make them excellent candidates for single molecule electronics. A family of derivatives with different electronic properties can be created by adding various functionalized side groups, which effect the conductance properties of the phenylene-ethynylene backbone. These derivatives with different electronic properties can be utilized to implement novel logic functions in nano circuits.

Here we present the results of a combined theoretical and experimental investigation of the adsorption characteristics, electronic structure and bonding geometry of single 1,4-bis(phenylethynyl)-2,5bis(ethoxy)benzene (PEEB) molecules on the Au(111) surface. DFT calculations of the density of states (DOS) and adsorption geometry were found to be in qualitative agreement with low temperature STM images and STS measurements. The strength of the bonding interaction to the substrate was also calculated.

# Unsaturated Metallic Lead Defect States in Layered Low Dimensional Hybrid Perovskite Quantum Wells

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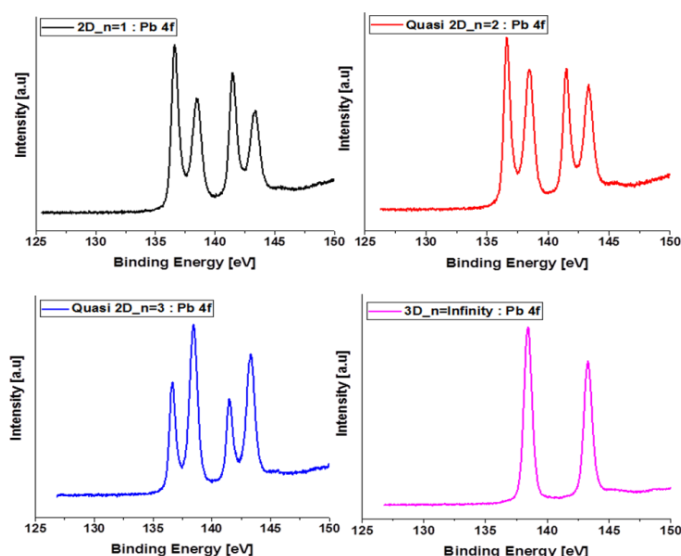
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Owing to its versatile photo-physical properties, layered two-dimensional (2D) hybrid perovskites exhibit a greater capacity in optoelectronics. A series of layered 2D, quasi 2D and 3D hybrid halide perovskites based on octyl, methyl and lead iodide with chemical formula of  $(C_8H_{20}N)_2PbI_4$ ;  $(C_8H_{20}N)_2(CH_3NH_3)Pb_2I_7$ ;  $(C_8H_{20}N)_2(CH_3NH_3)_2Pb_3I_{10}$  and  $CH_3NH_3PbI_3$  yielding to different layers  $n=1, 2, 3$  and  $\infty$  respectively were prepared. From our XPS studies we found the presence of unsaturated metallic lead states in 2D and quasi 2D perovskite thin films and we suspect that the presence of unsaturated Pb defect states in layered perovskites also played a key role in tuning the optoelectronic properties<sup>[1-3]</sup>. The shift of periodic peak in X-ray diffraction towards low  $2\theta$  values by increase in number of layers suggests the increase in quantum well thickness. Raman spectra reveal the highly ordered crystal structure movement in the layered perovskites containing both shorter and longer alkylammonium cation. The photo detectors based on  $n=1$ , 2D layered perovskite exhibited faster response time of 0.40s compared to 0.71s for 3D perovskites with very low dark currents ( $4.29 \times 10^{-10}A$ ).



**Figure1.** High resolution X-ray photoelectron spectra of Pb 4f for  $(C_8H_{20}N)_2PbI_4$  (2D),  $(C_8H_{20}N)_2(CH_3NH_3)Pb_2I_7$  (quasi 2D),  $(C_8H_{20}N)_2(CH_3NH_3)_2Pb_3I_{10}$  (quasi 2D) and  $CH_3NH_3PbI_3$  (3D) hybrid halide perovskites.

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# Functionalization of two-dimensional materials with polymer brushes

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**Abstract:** MoS<sub>2</sub> is one of the well-known two-dimensional (2D) materials owing to its unique structures, a wide range of chemical compositions, and a vast array of unique physical properties. However, dispersibility of MoS<sub>2</sub> has always been a great challenge and some applications of MoS<sub>2</sub> are limited due to its own structure. Functionalization of materials could facilitate the improvement of dispersibility and allow for the tuning of properties of 2D materials. Therefore, in this work, MoS<sub>2</sub> was modified with polymer brushes by a facile self-initiated photografting and photopolymerization (SIPGP) method to obtain functional MoS<sub>2</sub> materials. By the preparation of polymer brushes on MoS<sub>2</sub> surface, the thickness of functionalized MoS<sub>2</sub> was determined by atom force microscope (Figure 1). Meanwhile, functionalized MoS<sub>2</sub> also showed good dispersibility property in H<sub>2</sub>O. We hope that this simple way can improve the optical, electronic and chemical properties of MoS<sub>2</sub> materials and open more applications for 2D materials.

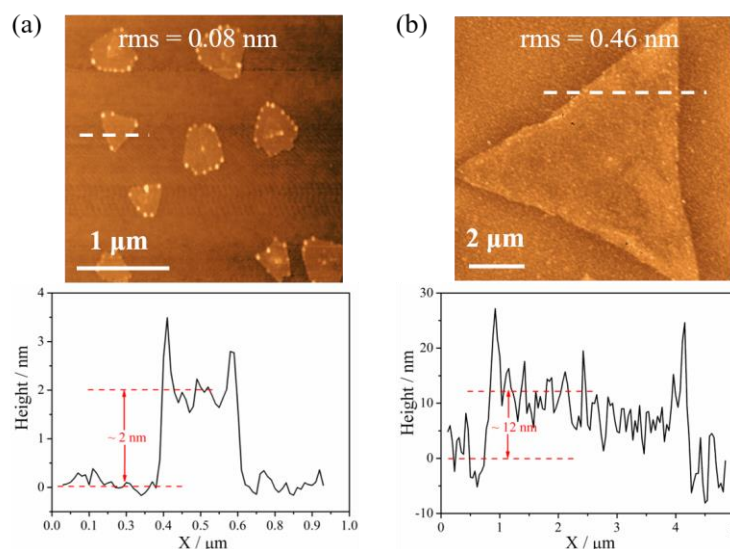


Figure 1. AFM height scan image of MoS<sub>2</sub> before (a) and after (b) SIPGP with PMMA.

# Low temperature MCBJ measurements of Buckminster - Fullerenes

Alexander Strobel<sup>1,2</sup>, Filip Kilibarda<sup>1,2</sup>, Tobias Böhler<sup>2</sup>, Elke Scheer<sup>2</sup>, Thomas Huhn<sup>2</sup>, Artur Erbe<sup>1,2</sup>

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The poster shows the electrical transport characteristics of C<sub>60</sub> Buckminster 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. Fragments of the C<sub>60</sub> Buckyball, so called Buckybowls acquire the important Fullerene feature, its curvature. Corannulene (C<sub>20</sub>), the smallest subunit of C<sub>60</sub>, is introduced as an interesting candidate for electronic transport measurements. 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.

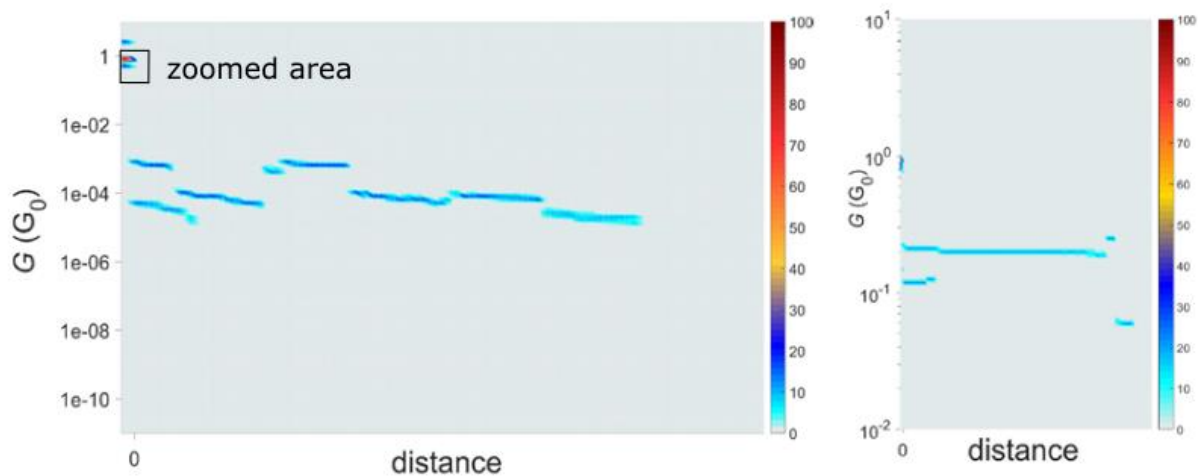


Figure 1: Conductance histogram of 15 opening curves at 10 K with the zoomed 0.1 G<sub>0</sub> state.

## Nano-electronic components built from DNA templates

Jingjing Ye<sup>1</sup>, Richard Weichert<sup>2</sup>, Seham Helmi<sup>1&</sup>, Alexander Eychmüller<sup>2</sup>, Ralf Seidel<sup>1</sup>

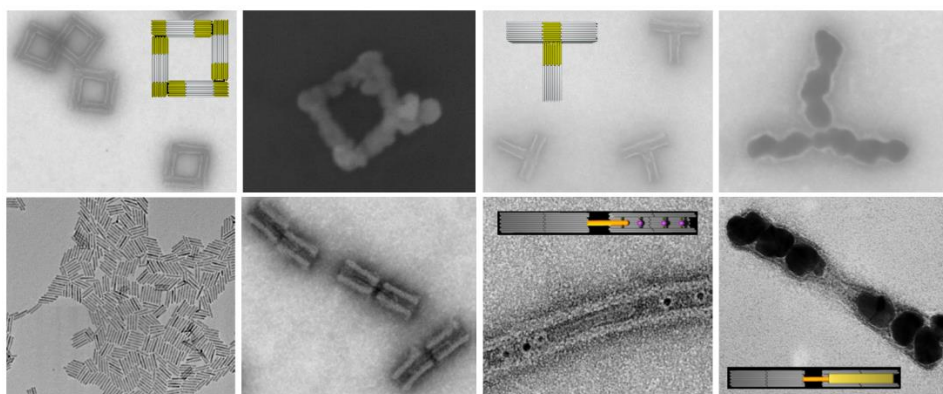
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On the nanoscale, fundamental properties and potential applications are greatly influenced by the size and shape of the material. “DNA Origami” takes advantage of base complementarity of individual short oligonucleotides, to fold a long “scaffold strand” into almost any continuous 2D or 3D shape.<sup>[1]</sup> We recently introduced a new concept of DNA origami 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  $\mu\text{m}$  long conductive gold nanowires with 20-30 nm diameters.<sup>[3]</sup> With conductance characterization, metallic conducting wires were demonstrated. Here the concept is further expanded by designing mold monomers with different geometries and interfaces. We can fabricate more complex ‘mold-superstructure’ in a unique and flexible way like lego bricks. We can also incorporate semi-conducting nanorods into this mold-based system for further single molecular transistor application. In addition, double-stranded DNA layer known for high spin-selectivity, incorporated in the metallic wire can also be used as efficient spin filter for spintronic applications.



Sketch and TEM (SEM) images showing the Lego®-Brick like nanostructure assembly

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# Zn-ion hybrid microsupercapacitors with ultra-high areal energy density and long-term durability

Panpan Zhang<sup>1,2</sup>, Yang Li<sup>3,4</sup>, Faxing Wang<sup>1,2</sup>, Gang Wang<sup>1,2</sup>, Sheng Yang<sup>1,2</sup>, Jian Zhang<sup>1,2</sup>, Feng Zhu<sup>3,4</sup>, Xiaodong Zhuang<sup>1,2</sup>, Oliver G. Schmidt<sup>2,3,4</sup> & Xinliang Feng<sup>\*1,2</sup>

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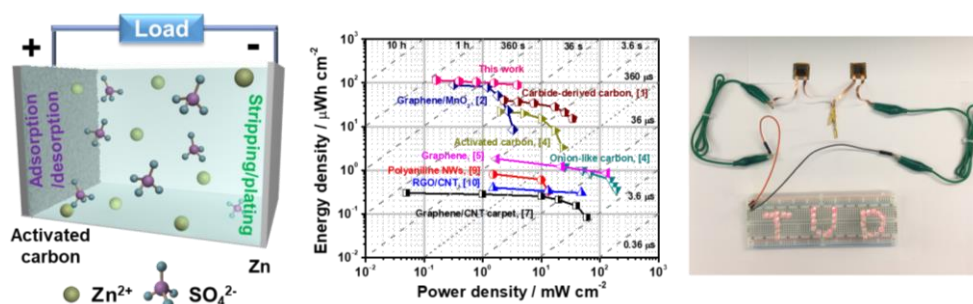
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Nowadays, most reported microsupercapacitors (MSCs) still suffer from the unsatisfied areal energy density ( $<10 \mu\text{Wh cm}^{-2}$ ), hindering their practical applications. Constructing a hybrid supercapacitor with a battery-type anode electrode and a capacitor-type cathode electrode has been an attractive method to achieve the merits from both rechargeable batteries and supercapacitors. In this respect, we demonstrate a new-type Zn-ion hybrid MSC with ultrahigh areal energy density and long-term durability, by employing activated carbon as a cathode electrode and electrodeposited Zn nanosheets as an anode electrode in  $\text{ZnSO}_4$  aqueous electrolyte. The areal capacitance reaches a record of over  $1200 \text{ mF cm}^{-2}$  at  $0.16 \text{ mA cm}^{-2}$  in a voltage range of  $0.5\text{-}1.5 \text{ V}$  and the areal energy density of up to  $115.4 \mu\text{Wh cm}^{-2}$  at a power density of  $0.16 \text{ mW cm}^{-2}$ , which are much higher than those of the state-of-the-art MSCs. Besides, the Zn-ion hybrid MSCs exhibit a superb cycling stability without noticeable decay after 10000 cycles. Thus, the Zn-ion hybrid MSCs with unique characteristics of such excellent reversible capacitance, high-rate capability, and good cycling performance will act as a new generation of miniaturized energy storage devices.



## **Your Notes**

## **Your Notes**

## Hiking Tour to the Gottleuba Blick (total 4.8km, 1:24h)

**A: Hotel Augustusberg,**

**1: turn to the right, take the path going upwards**

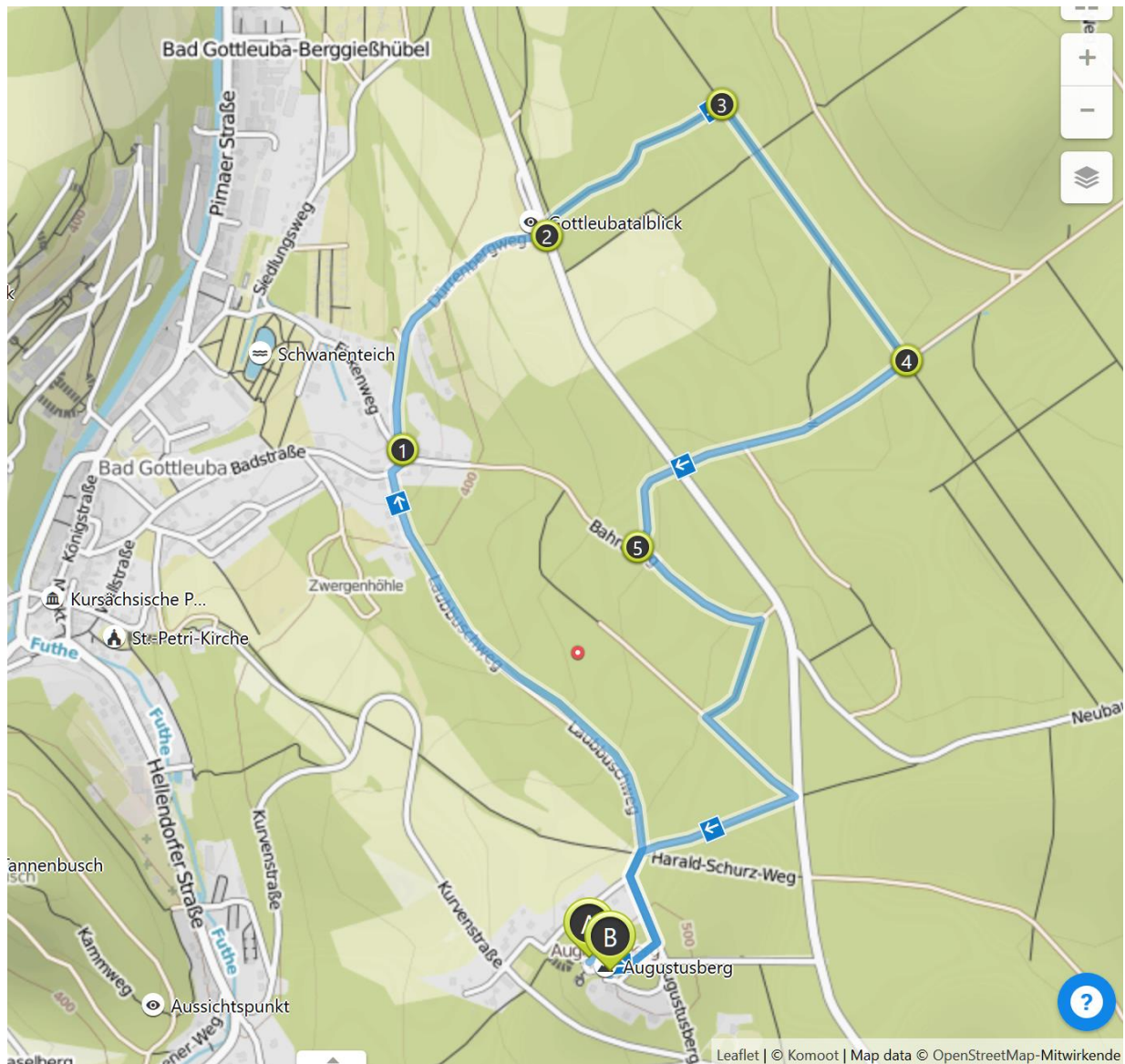
**2: View to the Gottleuba valley,** then cross the street at the old stone cross, follow the small path into the forest,

**3: turn right at a larger path,**

**4: turn right at a paved way,**

**5: turn left- upwards,**

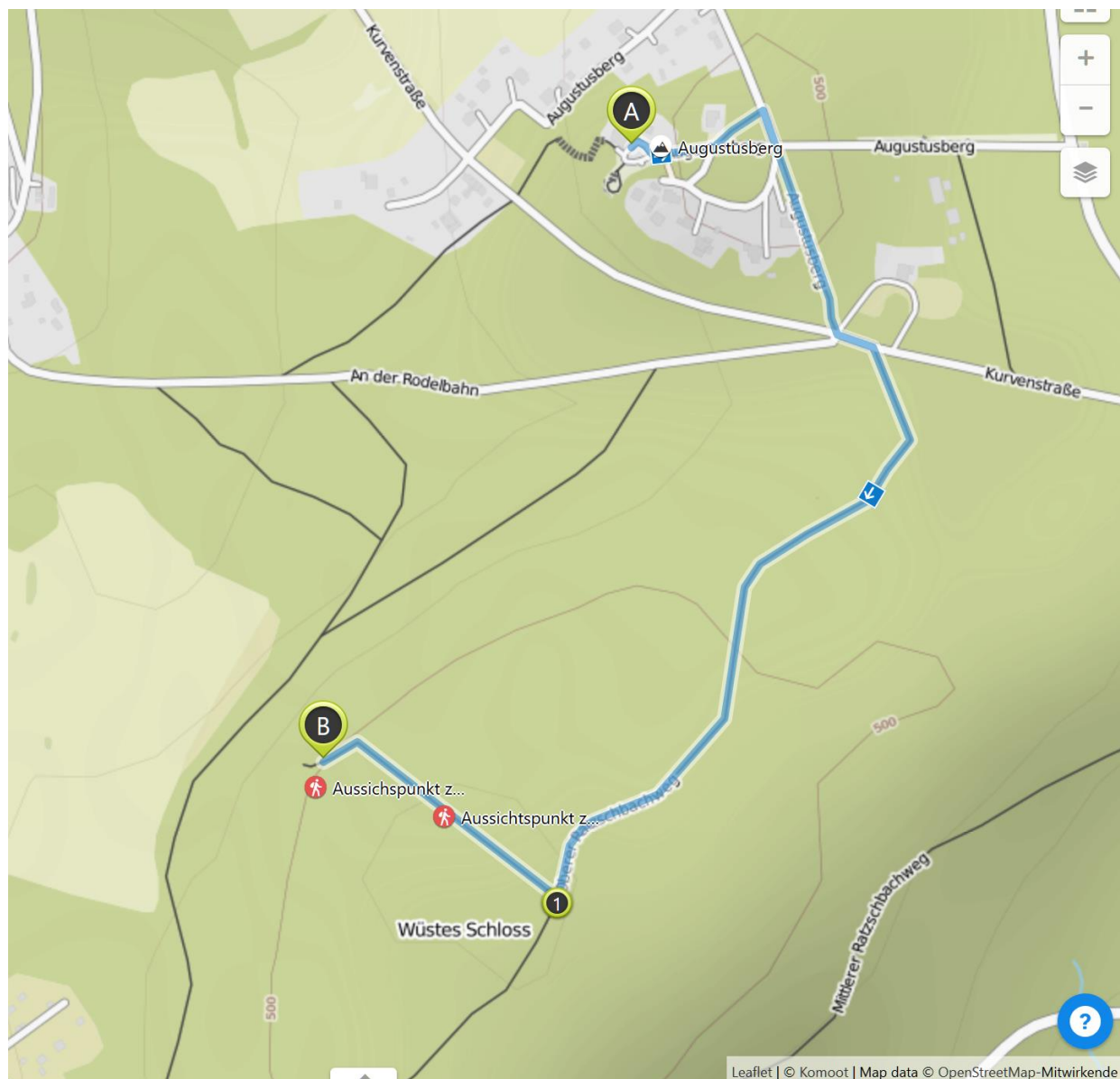
**B: You reached the dinner site.**



**Alternative: Walk to the Gottleuba Dam view (less attractive, total 2.8km, 0:46h)**

**A: Hotel Augustusberg**

**1: turn to the right, take the path until you reach the view point (B), with a glimpse to the Gottleuba Dam in western direction**



## NanoNet Annual Workshop 2018, Augustusberg

### Participants

Updated: 03.09.2018 (PZ)

Name	First Name	Gender	Title	Institution
Arora	Himani	Ms.		HZDR
Baek	Eunhye	Ms.		TU Dresden
Bayrak	Türkan	Ms.		HZDR
Davitt	Fionan	Mr.		UCC Cork
Ditte	Kristina	Ms.		IPF Dresden
Echresh	Ahmad	Mr.		HZDR
Erbe	Artur	Mr.	PD Dr.	HZDR
Garcia	Adria	Mr.		UCC Cork
Gemming	Sibylle	Mrs.	Prof. Dr.	HZDR
Georgiev	Yordan	Mr.	Dr.	HZDR
Günther	Florian	Mr.	Dr.	HZDR/TU Dresden
Jazawandi	Shima	Ms.		HZDR
Joachim	Christian	Mr.	Prof. Dr.	CEMES Toulouse
Jordan	Rainer	Mr.	Prof. Dr.	TU Dresden
Kelling	Jeffrey	Mr.		HZDR
Khan	Bilal	Mr.		HZDR
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Lissel	Franziska	Ms.	Dr.	IPF Dresden
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Metzger	Robert	Mr.	Prof. Dr.	U Alabama
Moresco	Francesca	Mrs.	Dr.	TU Dresden
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Strobel	Alexander	Mr.		HZDR
Voit	Brigitte	Mrs.	Prof. Dr.	IPF Dresden
Ye	Jingjing	Ms.		U Leipzig
Zahn	Peter	Mr.	PD Dr.	HZDR
Zhang	Panpan	Mr.		TU Dresden



**HZDR**

 **HELMHOLTZ**  
ZENTRUM DRESDEN  
ROSSENDORF

