

International Helmholtz Research School  
for Nanoelectronic Networks



# IHRS NANONET

## International Conference 2019

8 – 11 October 2019

Hotel INNSIDE by Melia, Dresden, Germany



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## Venue and organization

### Venue

Hotel INNSIDE by Melia  
Salzgasse 4  
01067 Dresden, Germany  
Phone: +49 351 79515-0, Fax: +49 351 79515-4099  
E-mail: [inside.dresden@melia.de](mailto:inside.dresden@melia.de)  
Homepage: [www.melia.com/Innside/Dresden](http://www.melia.com/Innside/Dresden)

### Organization

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

### Scientific Organizers

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

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

### Local Organizer

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

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

**Agenda**
 Place: Hotel Innside by Melia, Salzgasse 4, 01067 Dresden  
 updated: 05.10.2019 (PZ)
**Tuesday, 08 October 2019**

Start	Who	Durat.	Short Title (Full titles see next page)	Notes
12:00			Arrival/Lunch Buffet	Chair: Zahn, P.
13:30	Erbe, A.		Welcome address	
13:40	<b>Joachim, C.</b>	60+10	Nanocar Race I & II: Technology and Molecule-mechanics	
14:50	Strobel, A.	25+5	Electrical characterization of C60 molecules at low temperatures	
15:30		30	Break	Chair: Joachim, C.
16:00	<b>Herrmann, C.</b>	40+10	Spin-dependent effects: molecular + nanoscale electron transport	
17:00		120	<b>Poster session</b>	ca. 30 Posters
19:30			Dinner	at Hotel

**Wednesday, 09 October 2019**

Chair: Bol, A.

8:45	<b>Seifert, G.</b>	40+10	Layered Inorganic Nanostructures – Electronic and Structural Properties	
9:35	Arora, H.	25+5	Charge transport in two-dimensional materials	
10:15		30	Break	Chair: Kolesnik-G., M.
10:45	<b>Bol, A.</b>	40+10	ALD of TM di- and tri-chalcogenides with phase and morphology control	
11:35	Krstić, V.	25+5	Extended electronic boundaries in graphene: Dirac-Fermion-Optics	
12:20			<b>Conference Photo</b>	
12:30			Lunch	Chair: Arora, H.
14:00	<b>Ortmann, F.</b>	40+10	From Electronic Structure to Charge-, Spin- and Polaron-Transport	
14:50	Kolesnik-Gray, M.	25+5	Edge fluorinated graphene: Electronic properties of thin films and flakes	
15:20	Honolka, J.	25+5	Antiferromagnetic domain ordering processes in quasi-2D Fe-chalcogenide	
16:00		30	Break	
17:15			<b>Sightseeing – Walking Tour 2h</b> (start in front of the hotel)	
19:15			Free Time	

**Thursday, 10 October 2019**

Chair: Krstić, V.

8:45	<b>Frank, O.</b>	40+10	Deformation in 2D materials	
9:35	Khan, B.	25+5	Towards Reconfigurable Transistors: Rapid Thermal vs. Flash Lamp Annealing	
10:15		30	Break	Chair: Georgiev, Y.
10:45	<b>Holmes, J.</b>	40+10	Synthesis and Properties of Direct Bandgap Ge-Sn Nanowires	
11:35	Garcia, A.	25+5	Single-pot synthesis of metal-free group-IV semiconductor nanowires	
12:15			Lunch	Chair: Zhuravel, R.
13:45	<b>Kleinekathöfer, U.</b>	40+10	Environmental effects on energy and charge transfer in molecular systems	
14:35	Braun, H.-G.	25+5	Self organisation of peptides - Realise complex functional microstructures	
15:05	Bayrak, T.	25+5	Functionalized DNA Origami Nanostructures for Molecular Electronics	
15:45		30	Break	
17:30			<b>Steam Boat Tour</b> ("Meissen" from pier 1-7)	
- 22:00			<b>Conference Dinner</b> (Poster Prize)	on Boat

**Friday, 11 October 2019**

8:30			<b>Check-Out</b> (latest 12:00)	Chair: Zahn, P.
8:45	<b>Metzger, R.</b>	40+10	Unimolecular Electronics: Is there a Future?	
9:35	Moresco, F.	25+5	Model systems for atomic scale electronics	
10:15		30	Break	Chair: Erbe, A.
10:45	<b>Porath, D.</b>	40+10	Novel DNA-Based Molecules and Their Charge Transport Properties	
11:35	Zhuravel, R.	25+5	Backbone charge transport in ds-DNA	
12:05	Zessin, J.	25+5	Characterization of DNA-based Nanostructures for Nanoelectronics	
12:45			Lunch	
14:00			Departure	

Breakfast will be served from 06:30.

## NanoNet International Conference 2019, Dresden

### Talks

updated: 01.10.2019 (PZ)

Presenter	Title	Pg.
<b>Invited Talks</b>		
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Frank, O.	Deformation in 2D materials	4
Herrmann, C.	Spin-dependent effects in molecular and nanoscale electron transport: challenges for first-principles descriptions	5
Holmes, J.	Synthesis and Properties of Direct Bandgap Germanium-Tin Nanowires	6
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Arora, H.	Charge transport in two-dimensional materials	13
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Braun, H.-G.	Self organisation of peptides (FmocFF) - A versatile route to realise complex functional microstructures	15
Garcia, A.	Single-pot synthesis of metal-free group IV semiconductor nanowires	16
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Krstić, V.	Extended electronic boundaries in graphene: in the limit of high-covalently functionalised derivatives and Dirac-Fermion-Optics	20
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# ALD of Transition Metal Di- and Tri-Chalcogenides with Phase and Morphology Control

Ageeth A. Bol

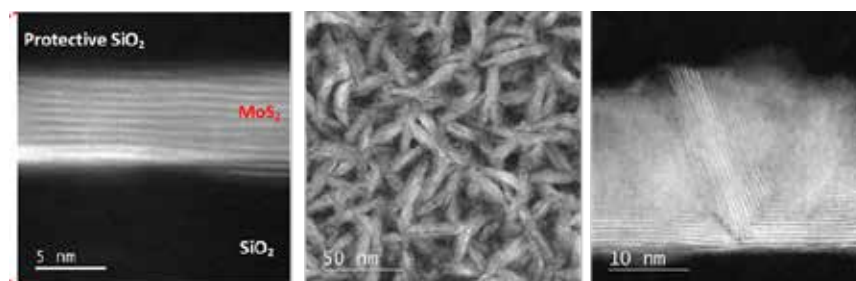
Dept. of Applied Physics, Eindhoven University of Technology, the Netherlands

Corresponding author: a.a.bol@tue.nl

2D materials have been the focus of intense research in the last decade due to their unique physical and chemical properties. This presentation will highlight our recent progress on the synthesis of two-dimensional transition metal di- and tri-chalcogenides (2DTMCs) for nanoelectronics and catalysis applications using atomic layer deposition (ALD). ALD-grown 2DTMC films typically exhibit a high density of out-of-plane 3D structures in addition to 2D horizontal layers. While the out-of-plane 3D structures are ideal for catalysis applications, the presence of such 3D structures can hinder charge transport, which hampers device applications. In this presentation I will show how we used mechanistic insight obtained by HRTEM and DFT simulations to tune the shape and density of the 3D structures during plasma-enhanced ALD. The obtained morphology control was further confirmed by electrocatalysis and electrical measurements.

In the second part of my talk I will demonstrate that we also can modulate the crystal phase of transition metal chalcogenides through ALD. Phase-control between the metallic  $\text{TiS}_2$  and semiconducting  $\text{TiS}_3$  phases was achieved by carefully tuning the co-reactant ( $\text{H}_2\text{S}$  gas vs plasma) and deposition temperature during ALD. These two material phases were differentiated using a variety of characterization techniques.

This work sets the foundation for achieving electrical and catalytic property modulation through phase and morphology control in low-dimensional materials during ALD.



*Figure 1: Various morphologies of  $\text{WS}_2$  obtained by tuning the ALD processing parameters. Pictures obtained by HAADF-STEM.*

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## Deformation in 2D materials

Otakar Frank<sup>1</sup>

<sup>1</sup>J. Heyrovsky Institute of Physical Chemistry of the CAS, Prague, Czech Republic

Corresponding author: otakar.frank@jh-inst.cas.cz

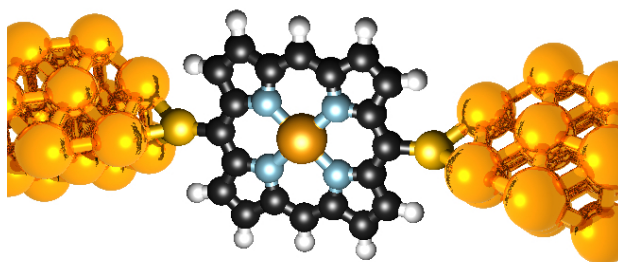
Mechanical deformation plays an important role in 2D materials because it causes drastic changes of their properties, ranging from (opto)electronic to magnetic, chemical, or mechanical ones. In-plane stress represents well documented and straightforward means of exerting not-so-severe, but reasonably controlled level of deformation. Fundamental considerations regarding the stress transfer from the substrate to the examined 2D material and the basics of monitoring the process by Raman spectroscopy will be given in the first part of the talk. In contrast, direct out-of-plane deformation (compression) can offer a very interesting and more effective route to modify the properties of 2D materials thicker than 1 atom, e.g. bilayer graphene or monolayer transition metal dichalcogenides, which will be briefly discussed in the second part. More importantly, from a different view point, out-of-plane deformation comprises also all kinds of topographical distortions like ripples, wrinkles, folds etc. These corrugations are almost omnipresent because of the low bending rigidity of 2D materials and they form and change readily upon even miniscule stress. The nanometer-sized ripples cause dramatic decrease of mobility. The larger wrinkles and folds can generate a plethora of effects like gauge fields, energy funneling, or quantum confinement. There is a dire need to control the appearance and dimensions of such structures. The final part of the talk will summarize our recent efforts of manipulating this “third dimension” of 2D materials, with the focus on (i) the interplay of graphene and a compliant supporting polymer, and (ii) locally supported graphene by nano-pillar arrays.

# Spin-dependent effects in molecular and nanoscale electron transport: challenges for first-principles descriptions

Carmen Herrmann<sup>1</sup>

<sup>1</sup>*Institute of Inorganic and Applied Chemistry, University of Hamburg, Martin-Luther-King-Platz 6, 20146 Hamburg, Germany, carmen.herrmann@chemie.uni-hamburg.de*

Using the spin degree of freedom offers fascinating options for nanoscale functionality, and also provides new data for improving our insight in fundamental aspects of nonequilibrium physics at that scale. For interpreting experimental data and for suggesting new experiments, theoretical simulations and concepts are often necessary. First-principles theoretical approaches have the advantage of being independent from system-specific fit parameters and therefore in principle predictive, but in practice, compromises between accuracy and computational feasibility imply that for molecular and nanoscale spintronics, a reliable first-principles description may be elusive [1]. We illustrate the resulting challenges as well as successes for examples such as chiral induced spin selectivity [2] and related spin-orbit effects [3], length-dependent charge delocalization in molecular wires [4], structure—property relationships for the Kondo effect of  $\text{Co}(\text{CO})_n$  molecules on a Cu surface [5,6].



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# **Synthesis and Properties of Direct Bandgap Germanium-Tin Nanowires**

Justin D. Holmes

School of Chemistry, University College Cork, Cork, Ireland

Alloying group-IV semiconductors (such as Ge or Si) with group-IV metals (such as Sn and Pb) can potentially lead to direct bandgap semiconductors, analogous to III-V materials, but with the distinct advantage over III-Vs of being Si compatible. A direct bandgap group-IV semiconductor would find applications in both optoelectronic, e.g. mid-IR photodetectors, and electrical, e.g. tunnel field-effect transistor (TFET) devices. However, due to the lattice mismatch between Ge and Sn, GeSn thin films often experience large amounts of strain. Compressive strain shifts the energy gap to lower wavelengths, therefore in order to achieve a direct bandgap a high Sn concentration is required, which can be difficult to accomplish. A promising solution to overcome the strain induced in GeSn thin films is to move towards GeSn nanostructures; a nanowire morphology allows increased strain relaxation compared to thin films due to free sidewall facets. In this presentation, I will give a brief overview of the recent advances in the synthesis of GeSn nanowires, including some of their optical and electrical properties.

# Nanocar Race I & II: Technology and Molecule-mechanics

Christian Joachim<sup>1,2</sup>

<sup>1</sup>CEMES-CNRS, Université de Toulouse, 29 rue Jeanne Marvig, 31055 Toulouse, France

<sup>2</sup>MANA-NIMS, 1-1 Namiki, Tsukuba, Ibaraki 305-0044, Japan

Corresponding author: [joachim@cemes.fr](mailto:joachim@cemes.fr)

## Abstract:

In 2013, we proposed the organization of a molecule-car race with different molecule-vehicles driven one by one, at the same time, by pilots using different scanning tunneling microscopes (STM) but on the same surface [1]. This was one consequence of a long period of research on single molecule mechanics started with the first observation of a single molecule in rotation [2] and followed by the construction of a few molecule(s) machinery like the single molecule-wheelbarrow [3], the molecular rack and pinion [4], the controlled rotation of a single molecule-rotor [5] and the first observation that a single molecule alone has enough power to rotate one way a few atoms [6] or another molecule [7].

With about 100 atoms, a molecule-vehicle has a chassis equipped with spacer chemical groups to hold it a few angstrom away from the surface, paddles, switchable legs or wheels and a motorization embedded on board [1]. For this first edition, pushing its molecule-vehicle using the known pushing, pulling or sliding STM manipulation modes was forbidden forcing each team to play with inelastic tunneling effects for a drive on the Au(111) surface [8]. The 27<sup>th</sup> of April 2017 at 11:00 am, the departure flag was up in the Toulouse control room with the 6 selected teams on their starting atomic line, ready to nano-race. The anticipated run was 100 nm on a single Au(111) surface with 2 turns. After 2 days and one night of intense efforts, the 29<sup>th</sup> of April 2017 at 17:00 pm, the first ever international nano-car race was a success. We will describe the UHV technologies created on purpose for this race involving in particular a unique LT-UHV 4-STM i.e. a scanning tunneling microscope with 4 scanners able to scan on the same surface and a special UHV sublimation system with a dedicated masking set-up. We will present some of the peculiar nano-car race sequences recorded during those 36 hours.

In 2018, we have announced the nano-car race second edition for spring 2021 organized under the MEMO (Mechanics with molecule(s)) European project. Eleven teams from all over the world are already officially registered [9]. The rules of this second edition will be given in a way to attract more teams to join the fun of designing, synthesizing and operating a single molecule machinery on a surface.

## References

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## **Environmental effects on energy and charge transfer in molecular systems: A multi-scale approach**

Ulrich Kleinekathöfer

Jacobs University Bremen, Dept. of Physics and Earth Sciences, Bremen, Germany

Email: u.kleinekathoefer@jacobs-university.de

Charge as well as excitation energy transfer processes are important and ubiquitous in many biological and manmade systems but at the same time complicated to model at the molecular level. In a multi-scale approach (classical) molecular dynamics simulations and electronic structure calculations will be combined. The results of such a treatment can subsequently be employed in quantum approaches to determine the respective charge and energy transfer scenarios as well as optical responses. As examples, the charge transport through a DNA molecule is detailed with a special emphasis on the time-dependent effects caused by the liquid environment.

Concerning the quantum transport through molecular wires, several theoretical approaches rely on assuming a molecule-lead coupling composed of Lorentzian functions and a decomposition of the Fermi function in connection with quantum master equations, hierarchical schemes or non-equilibrium Green's functions. The underlying assumptions make this strategy very unattractive due to the limitations in the form of the molecule-lead coupling and its inefficiency at low temperatures. To overcome these restrictions, a Chebyshev expansion is applied to derive a set of coupled ordinary differential equations within the non-equilibrium Green's functions formalism. The new scheme has been tested for molecular junctions under the influence of strong time-dependent perturbations leading, for example, to coherent destruction of tunneling.

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# Unimolecular Electronics: is there a Future?

Robert M. Metzger  
Laboratory for Molecular Electronics  
Department of Chemistry and Biochemistry  
University of Alabama, Tuscaloosa, AL 35487-0336, USA

Corresponding author [rmetzger@ua.edu](mailto:rmetzger@ua.edu)

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 (iii) the increases in device speeds in commercial inorganic integrated circuits as the device dimensions were halved every 18 to 24 months [2]

The first organic rectifier was measured in England and verified in Alabama in the 1990s. UME has matured [4,5]: its Ansatz was that single molecules with “electroactive properties” as one-electron donors D or as one-electron acceptors A, when properly configured in space 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 pn or np rectifiers or even npn’ transistors. Where are we now [3],[4]?

- (A) With massive corporate funding the race to the bottom, e.g. to 10 nm device half-pitch, was **won** by the semiconductor industry (Intel, Samsung, etc.).
- (B) Excited molecules could decay by photon emission instead of 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 [5].
- (D) If the variability in currents across each metal/molecule interface vastly exceeds 5%, **UME will have failed**. Maybe the groups of Nijhuis [5,6,7], Frisbie [8], and Batista [9], or others, will make crucial UME progress.

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# From Electronic Structure to Charge-, Spin- and Polaron-Transport

Frank Ortmann<sup>1</sup>

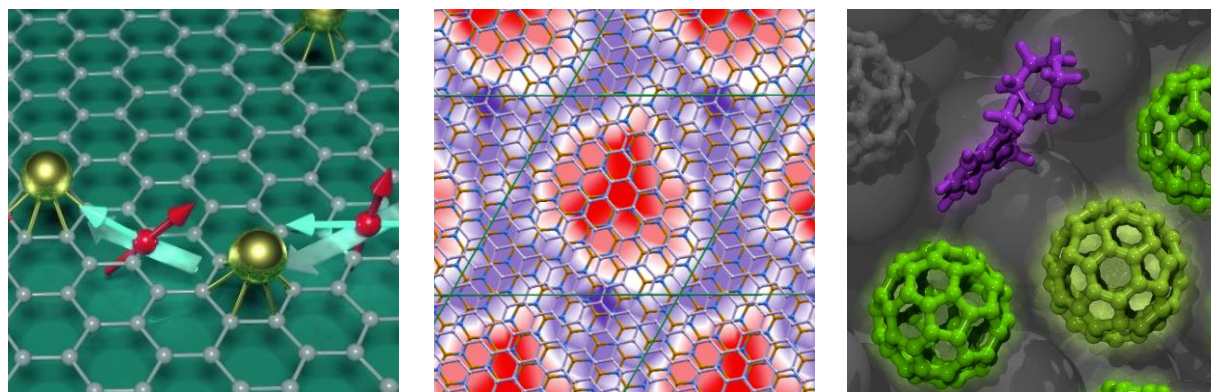
<sup>1</sup>Center for Advancing Electronics Dresden, Technische Universität Dresden,  
01062 Dresden, Germany

Corresponding author: frank.ortmann@tu-dresden.de

The number of materials in research is exploding and completely new classes are emerging that were unknown a few years ago, including topological insulators, Weyl semimetals, 2D materials and novel organic semiconductors. For such emerging materials, many computer codes easily implement theoretical approaches based on density function theory or many-body perturbation theory to describe electronic properties, which can be directly compared with measurements from angle-resolved photoelectron spectroscopy.

However, understanding charge transfer properties is much more complicated. This is because – in addition to electronic bulk properties – it requires describing disorder or other perturbations that are invisible to spectroscopic probes. In addition, typical transport geometries require the simulation of large systems, since the transport properties depend on the size of the system. Unfortunately, current tools either suffer from a lack of accuracy or scale badly with the system size.

In this presentation, I will introduce a linear-scaling approach that aims at closing this gap. For selected cases, I will demonstrate how large-scale charge-transport and spin-transport simulations based on the Kubo method in combination with electronic-structure simulations can lead to an in-depth understanding of various transport signatures that would otherwise remain unexplained.



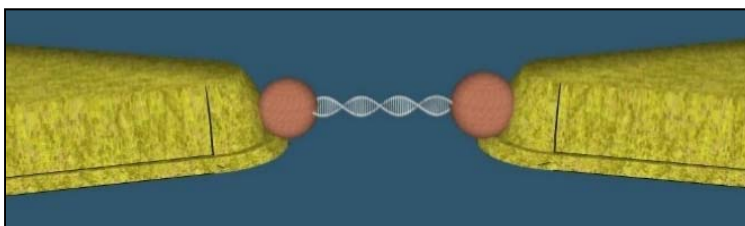
**Figure 1: Illustration of spin dependent transport in gold decorated graphene (left), the effective electrostatic potential of h-BN in a bilayer with graphene (middle) and the structure of an organic semiconductor blend (right).**

# Novel DNA-Based Molecules and Their Charge Transport Properties

**Danny Porath**

Institute of Chemistry and Center for Nanoscience and Nanotechnology, The Hebrew University of Jerusalem, 91904 Israel

danny.porath@mail.huji.ac.il



Charge transport through molecular structures is interesting both scientifically and technologically. To date, DNA is the only type of polymer that transports significant currents over distances of more than a few nanometers in individual molecules. Nevertheless and in spite of large efforts to elucidate the charge transport mechanism through DNA a satisfying characterization and mechanistic description has not been provided yet. For molecular electronics, DNA derivatives are by far more promising than native DNA due to their improved charge-transport properties.

In recent years we have invested great efforts to address the above issues. Measuring the charge transport in DNA was elusive due to great technical difficulties leading to various results. We recently devised an experiment in which double-stranded DNA is well positioned between metal electrodes. Electrical measurements give surprisingly high currents over 100 base-pairs (~30 nm) elevated from the surface. The temperature dependence indicates backbone-related band-like transport.

In collaboration with the Kotlyar group, We were also able to synthesize and measure long (hundreds of nanometers) DNA-based derivatives that transport significant currents when deposited on hard substrates. Among the molecules, metal containing DNA, which is true metal-organic hybrid, a smooth and thin metal coated DNA and G-quadruplex DNA.

## Layered Inorganic Nanostructures – Electronic and Structural Properties

Gotthard Seifert<sup>1</sup>, Jens Kunstmann<sup>1</sup>, Pavel Sorokin<sup>2</sup>, Zakhar Popov<sup>2</sup>

<sup>1</sup>Theoretical Chemistry, TU Dresden, Dresden, Germany

<sup>2</sup>National University of Science and Technology, MISIS, 119049 Moscow, Russia

Corresponding author: gotthard.seifert@tu-dresden.de

In addition to graphene, 2D transition-metal chalcogenides (e.g., MoS<sub>2</sub> and WS<sub>2</sub>), 2D modifications of phosphorus and many more single layers of layered materials have been studied theoretically as well as experimentally in recent years. Especially their electronic properties were investigated thoroughly due to the potential for application of such materials in future electronics. Much less studied was the magnetism of 2D structures. Here we present a family of layered structures with a high-spin atomic ground state, which exhibit ferromagnetic (FM) or anti-ferromagnetic (AFM) intra-layer ordering. These are Metal phosphorus trichalcogenides (MPT) of the formulae MPX<sub>3</sub>, with X=S(Se) and a broad variety of 3d-transition metals, but also – non-magnetic - main group metals (e.g. Mg, Zn). The results of DFT calculations and model calculations for magnetic properties will be shown.

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# Charge transport in two-dimensional materials

Himani Arora

Institute of Ion Beam Physics and Materials Research, HZDR, 01328 Dresden, Germany

Corresponding author: h.arora@hzdr.de

Here we report electronic characterization of few-layered Indium Selenide (InSe) and Gallium Selenide (GaSe), van der Waals semiconductors from the family of the III-VI chalcogenides. To tackle their instability under ambient conditions, an hBN-based encapsulation technique is discussed. After full hBN encapsulation, the devices show better FET performance and long-term stability as compared to unencapsulated devices. The full encapsulation of InSe(GaSe) flakes gives us an opportunity to understand their transport mechanisms in greater details [1].

In the second part, electronic and opto-electronic properties of a novel 2D semiconducting metal-organic framework(MOF) with the formula  $\text{Fe}_3(\text{THT})_2(\text{NH}_4)_3$  (THT=2,3,6,7,10,11-hexathiolotriphenylene) are discussed. We demonstrate for the first time band-like charge transport in MOFs using Hall-effect measurements. A record mobility of  $230 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$  at room temperature is obtained in  $1.7 \mu\text{m}$  thick MOF films. Subsequently, proof-of-concept photodetectors are fabricated with  $\text{Fe}_3(\text{THT})_2(\text{NH}_4)_3$  as an active element. The photodetectors demonstrate broadband photodetection in UV–NIR region; in addition, show a stable and reproducible photo-switching characteristics [2–3].

[1] Arora, H. et al., Effective hexagonal boron nitride passivation of few-layered InSe and GaSe to enhance their electronic and optical properties; *ACS Appl. Mater. Interfaces* (Submitted).

[2] Dong, R. et al., High-mobility band-like charge transport in a semiconducting two-dimensional metal–organic framework; *Nature Materials* **2018**, 17, 1027–1032.

[3] Arora, H. et al., Demonstration of a UV–NIR photodetector based on two-dimensional metal-organic frameworks (in preparation).

# Functionalized DNA Origami Nanostructures for Molecular Electronics

Türkan Bayrak<sup>1</sup>, Jingjing Ye<sup>2</sup>, Richard Weichelt<sup>3</sup>, Amanda Reyes<sup>4</sup>,  
Alexander Eychmüller<sup>3</sup>, Enrique Samano<sup>4</sup>, Ralf Seidel<sup>2</sup>, Artur Erbe<sup>1</sup>

<sup>1</sup>Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany.

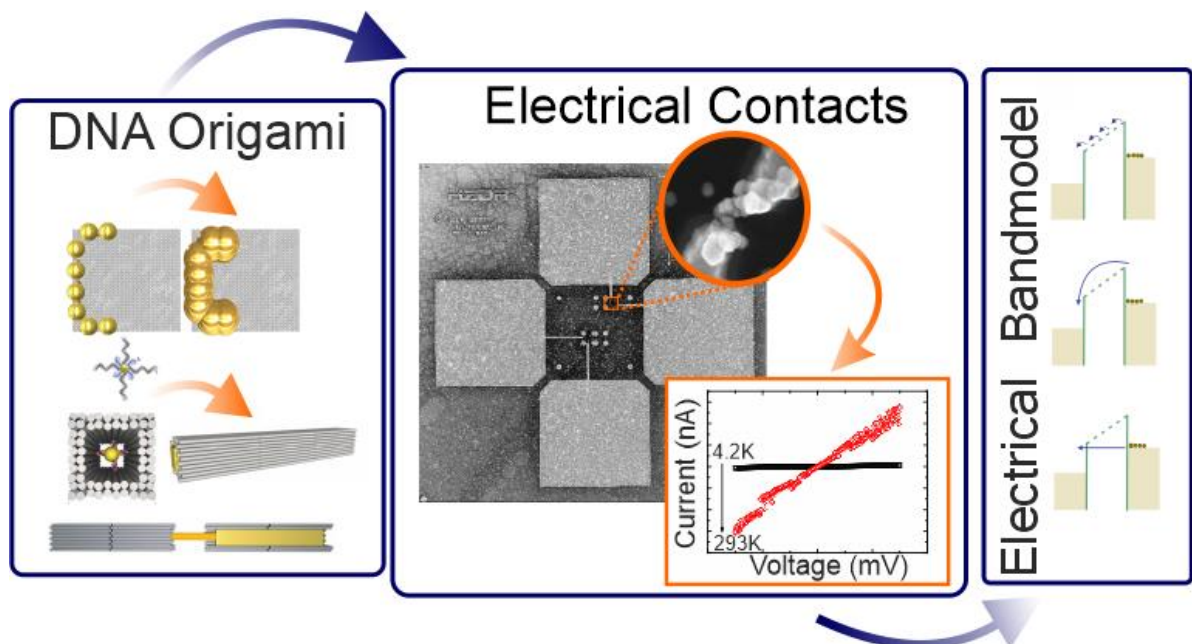
<sup>2</sup>Peter Debye Institute for Soft Matter Physics, Universität Leipzig, Germany.

<sup>3</sup>Physikalische Chemie, Technische Universität Dresden, Germany.

<sup>4</sup>Centro de Nanociencias y Nanotecnología, UNAM, Ensenada, Mexico.

Corresponding author: a.erbe@hzdr.dr

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 device fabrications. Based on this technique, the precise positioning of metallic and semiconducting nanoparticles along DNA nanostructures can be achieved. In this study, various DNA origami nanostructures (nanomolds, nanotubes and nanosheets) are used for the fabrication of nanoelectronic devices. To this end, gold nanoparticles, semiconductor quantum dots/rods are used in/on the DNA origami structures to create nanowires and transistor-like devices. The DNA origami nanowires and transistors were electrically characterized from room temperature (RT) down to 4.2K. Temperature-dependent characterizations of wires were performed in order to understand the dominant conduction mechanisms. Some nanowires showed pure metallic behavior. Transistor like devices showed Coulomb blockade at RT. The study shows that self-assembled DNA structures can be used for nanoelectronic patterning and single electron devices.



# Self organization of peptides (FmocFF) A versatile route to realize complex functional structures

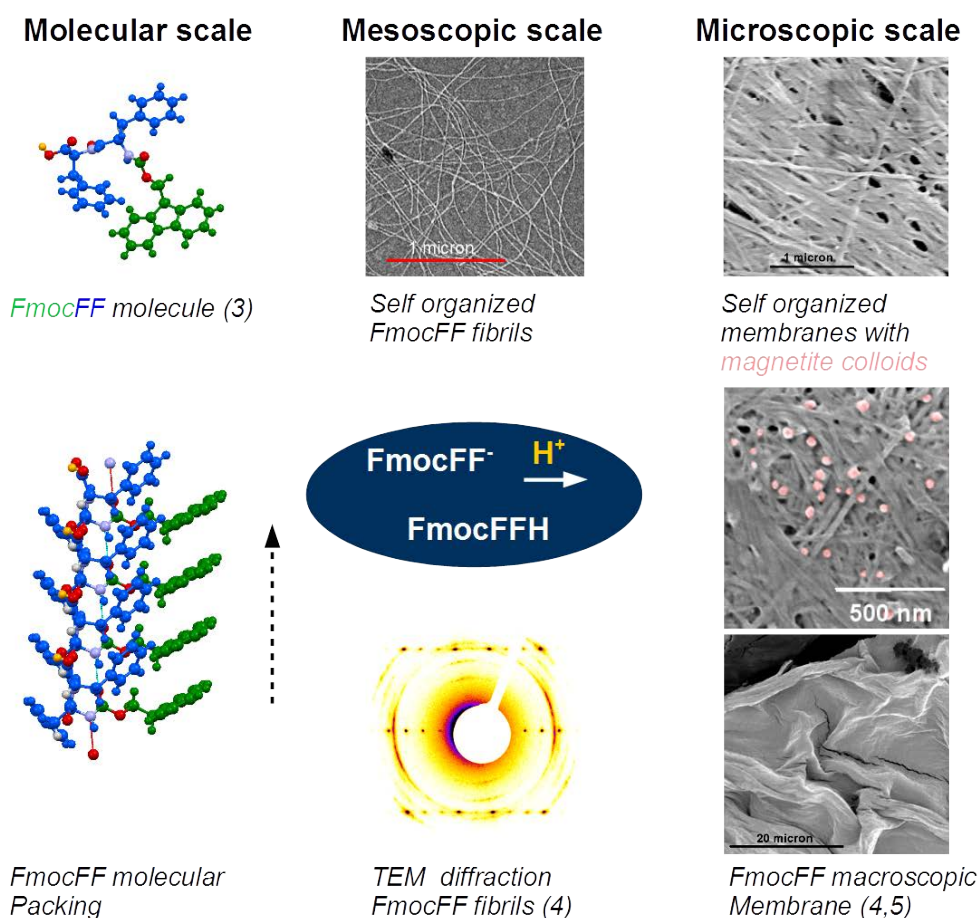
H.-G. Braun<sup>1,2</sup>, R. Goswami<sup>1,2</sup>, T. Sundaram<sup>1,2</sup> S. Banerjee<sup>1,2</sup>

<sup>1</sup>IPF Dresden, Dresden, Germany

<sup>2</sup>BIOTEC, TU Dresden, Dresden, Germany

Corresponding author: Hans-Georg.Braun@tu-dresden.de

The controlled self organization of appropriate DNA matrices and predefined oligo-DNA known as DNA origami has become a powerful strategy in bottom-up nanobiotechnology. Oligopeptides in particular those with aromatic groups have also become an interesting group of organic materials showing unusual properties as strong piezoelectricity for example (FmocFF) but the prediction of a variety of supramolecular nano-, meso- or microstructures (fibrils, ribbons, twisted ribbons, nanosheets, particles) is far less developed than for DNA origami. Some typical nano-, meso- and microstructures of FmocFF as generated by pH controlled self organization of small molecules in extended supramolecular structures will be discussed.



# Single-pot synthesis of metal-free group IV semiconductor nanowires

Adrià Garcia<sup>1</sup>, Subhajit Biswas<sup>1</sup>, Justin D. Holmes<sup>1</sup>

<sup>1</sup>School of Chemistry, University College Cork, Cork, Republic of Ireland

Corresponding author: 116223439@umail.ucc.ie

Catalytic three-phase bottom-up growth is the most popular method to generate germanium and silicon nanowires (NWs). However, the metal catalysts (e.g. Au, Ag, Ni, etc.) in this process can contaminate the semiconductor material to alter or deteriorate the properties to the NWs.

In this work, we report a simple, rapid and cost-effective synthesis approach for the self-seeded growth of Ge, Si and GeSn (11 at.% Sn) NWs through high-pressure solvothermal-like technique using low-boiling point solvents (e.g. toluene) and commercially available Si and Ge precursors (e.g. diphenylgermane). The NWs have high-aspect-ratio with diameter around 10 nm and are highly-crystalline. Control over the phase (cubic or tetragonal) of the nanowires was further achieved by altering the growth constraints such as temperature, pressure, precursor concentration, etc. Grown Ge nanowires demonstrated great efficiency as anode material in Li-ion battery with high specific capacity ( $\approx 1200$  mAh/g) and exceptional capacity retention.



# Antiferromagnetic domain ordering processes in quasi-2D Fe-chalcogenide van der Waals crystals

Jan Fikáček<sup>1</sup>, Jonas Warmuth<sup>2</sup>, Sunil Wilfred<sup>3</sup>, Cinthia Piamonteze<sup>4</sup>, Martin Bremholm<sup>5</sup>, Jan Minár<sup>4</sup>, Ján Lančok<sup>1</sup>, Philip Hofmann<sup>5</sup>, Jens Wiebe<sup>2</sup>, and Jan Honolka<sup>1</sup>

<sup>1</sup>Center for Analysis of Functional Materials, Institute of Physics of Czech Academy of Sciences, Na Slovance 1999/2, 182 21 Prague 8, Czech Republic

<sup>2</sup>Department of Physics, Hamburg University, Hamburg, Germany

<sup>3</sup>New Technologies Research Centre, University of West Bohemia, Plzeň, Czech Republic

<sup>4</sup>Paul Scherrer Institut, Forschungsstrasse 111, 5232 Villigen PSI, Switzerland

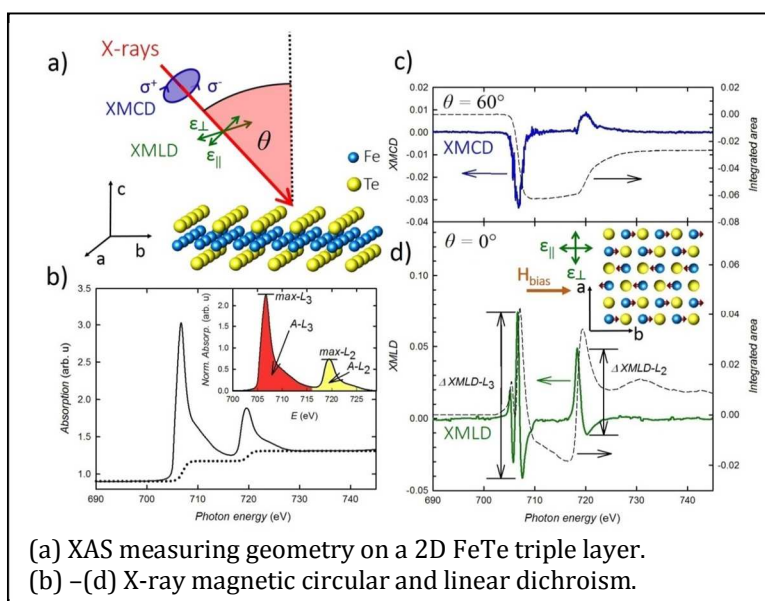
<sup>5</sup>Department of Chemistry, University of Aarhus, Aarhus, Denmark

Corresponding author: honolka@fzu.cz

Fe(Se,Te) type superconductors (SCs) are quasi two-dimensional (2D) van-der-Waals stacked crystals with a layer unit cell thickness of  $\sim 3\text{\AA}$ . Their Cooper pairing mechanism is believed to be *unconventional*, i.e. not phonon-mediated with critical temperatures  $T_c = 8\text{ K}$  in the case of bulk FeSe. Generally, the physics of *unconventional* SC is not understood but is believed to be intimately connected to non-local fluctuations of either *spin* or charge degrees of freedom [1].

Here we give an overview of temperature dependent structural and magnetic phase transition studies in FeTe. Contrary to FeSe, FeTe is not superconducting and orders antiferromagnetically (AFM) below 80 K. Its magnetic structure and ordering temperature depends on the amount of iron excess [2,3]. Interestingly, mixed alloys  $\text{FeTe}_{1-x}\text{Se}_x$  are superconducting with  $T_c$  higher than those of pure FeSe ( $T_c = 14.5\text{ K}$  at  $x = 0.5$ ). Thus, also the understanding of magnetism and electronic properties of FeTe is important as to reveal the origin of superconductivity in Fe-chalcogenides. For this, we conducted X-ray absorption spectroscopy (XAS) experiments at the Swiss Light Source in Villigen on Fe-rich  $\text{Fe}_{1+x}\text{Te}$  single crystals. Using different photon polarizations, we track X-ray magnetic circular dichroism (XMCD) and X-ray magnetic linear dichroism (XMLD) versus temperature, while FeTe enters the AFM state below  $T_N \sim 70\text{ K}$ . The data is compared to density functional theory calculations and results are discussed in view of effects in AFM domain dynamics.

\*This work was supported by the Czech Science Foundation Grant No. 19-13659S



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- [2] J. Warmuth et al., Quantum Materials **3**, 21 (2018)
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# Towards Scalable Reconfigurable Transistor Fabrication: Flash Lamp Annealing for Nickel Silicidation of Silicon Nanowires

Muhammad Bilal Khan<sup>1,2</sup>, Slawomir Prucnal<sup>1</sup>, René Hübner<sup>1</sup>, Artur Erbe<sup>1</sup>, Yordan M. Georgiev<sup>1,3</sup>

<sup>1</sup> Institute of Ion Beam Physics and Materials Research, HZDR, Dresden, 01328, Germany

<sup>2</sup> International Helmholtz Research School for Nanoelectronic Network, HZDR, Dresden, 01328, Germany

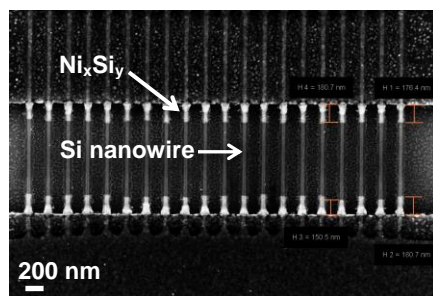
<sup>3</sup> On leave of absence from the Institute of Electronics at Bulgarian Academy of Sciences, 72, Tsarigradsko chausse blvd., Sofia, 1784, Bulgaria

Corresponding author: m.khan@hzdr.de

To complement scaling of field effect transistors, new device concepts have been introduced. One such concept is the reconfigurable field effect transistor (RFET). These transistors are based on nickel silicide-Si-nickel silicide Schottky junctions and their polarity can be switched between *p*- and *n*- type at runtime by the application of an electrostatic potential [1]. Control over silicide length and phase is important for scaling and proper functioning of these devices [2]. NiSi<sub>2</sub> is the desirable silicide phase as it yields similar Schottky barriers for electrons and holes, which enables reconfigurability of the device [1, 3].

We report on fabrication and electrical characterization results of RFETs. Si nanowires (SiNWs) are fabricated on undoped silicon-on-insulator (SOI) substrates by a top-down process based on electron beam lithography and inductively coupled plasma etching. Then, Ni is placed at both ends of the SiNWs by metal evaporation and lift-off processes. Afterwards, flash lamp annealing (FLA) is performed for silicidation of the NWs.

FLA has enabled better control over silicidation length. FLA process is much shorter (of the order of milli-seconds) than rapid thermal annealing process. Transmission electron microscopy shows the formation of the desired NiSi<sub>2</sub> phase near the silicide-Si interface. Electrical characterization of the devices with back gating shows ambipolar behaviour.



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## Edge fluorinated graphene: Impact of F content on the electronic properties of thin films and individual flakes

Maria Kolečnik-Gray<sup>1</sup>, Vitalii I. Sysoev<sup>2</sup>, Stefan Gollwitzer<sup>1</sup>, Dmitry V. Pinakov<sup>2</sup>, Galina N. Chekhova<sup>2</sup>, Lyubov G. Bulusheva<sup>2</sup>, Alexander V. Okotrub<sup>2</sup>, and Vojislav Krstić<sup>1</sup>

<sup>1</sup>Department of Physics, Friedrich-Alexander Universität Erlangen-Nürnberg (FAU),  
91058 Erlangen, Germany

<sup>2</sup>Nikolaev Institute of Inorganic Chemistry SB RAS, Novosibirsk State University,  
630090 Novosibirsk, Russian Federation

Corresponding author: vojislav.krstic@fau.de

Covalent fluorination has been of continued interest as means to introduce novel electronic transport functionalities in graphene derivatives. The high electronegativity of fluorine opens various possibilities towards the functional electronic modification of graphene for devices.

We study the electronic properties of graphene fluorinated at room temperature, with F content ranging from 2.4 to 16.6 at%. Depending on the device architecture, the electrical properties of fluorinated graphene (FG) devices were found to be significantly different: The electrical conductivity of thin films consisting of FG flakes decreases by several orders of magnitude with increasing F content. In contrast, individual flakes show a significant increase in both conductivity and carrier mobility. These results point towards the presence of edge-functionalization: while the conductivity of thin films is dominated by the edge-to-edge and edge-to-flake junctions, the individual flakes are doped remotely by F saturating the edges of the (undisrupted) graphene. This has been further confirmed by Raman and XRD analysis. Our results show that the electrical properties of few- and monolayer fluorinated graphene (FG) can be modified in a controllable manner in order to tailor its electrical conductivity towards specific applications.

# **Extended electronic boundaries in graphene: in the limit of high-covalently functionalized derivatives and Dirac-Fermion-Optics**

Vojislav Krstić

Department of Physics, Friedrich-Alexander-Universität (FAU) Erlangen-Nürnberg, 91058  
Erlangen, Germany

Corresponding author: [vojislav.krstic@fau.de](mailto:vojislav.krstic@fau.de)

Electronic boundaries introduced deliberately into any material is a key-ingredient for the successful control of its electronic and optoelectronic properties. Graphene, however, consists structurally of two triangular sublattices with a unit-cell with two inequivalent carbon atoms. In particular, the low-energy electronic dispersion relation resembles the one of light. Therefore, (extended) electronic boundaries can lead to many different flavors regarding the (opto)electronic response of graphene-based devices.

Here we compare two types of extended electronic boundaries, one driven by covalent functionalization, the other promoted by physisorbed metals:

In the limit of high degrees of covalent functionalization the question arises to which extent graphene shows still an optoelectronic response with graphene-typical features. Associated with this question is the observed, yet unresolved, peak intensity enhancement with increase of  $sp^3$  carbon in virtually all optical responses. To elucidate this general phenomenon we present a phenomenological model accounting for the possible formation of confined  $\pi$ -conjugated domains surrounded by  $sp^3$  carbon regions. Our model is underpinned by combined Raman and electrical transport measurements.

Physical electronic boundaries use potentials rather than chemical (lattice-disrupting) modifications of the material. Thus, keeping the light-like nature of the charges in graphene gives rise to their caustic motion within sufficiently extended potentials unlike for materials with quadratic dispersion relation. This unique propagation is source for a guiding of charges (through scattering), a cornerstone of Dirac-Fermion-Optics devices, which we will exemplify on the electronic analogue of the well-known Mie scattering in graphene exposed to periodically arranged extended potentials.

## **Model systems for atomic-scale electronics**

Frank Eisenhut, Dmitry Skidin, Justus Krüger, Tim Kühne, Francesca Moresco

cfaed, TU Dresden, 01062 Dresden, Germany

For the miniaturization of electronics down to atomic scale it is of fundamental importance to study molecular devices and atomic-size interconnections in a planar geometry. In this respect, scanning tunneling microscope (STM) experiments permit a deep insight into the electronic properties of molecular and atomic systems. Furthermore, on-surface synthesis is presently developing as a powerful strategy for the generation of complex functional molecules on a surface and opens new perspectives for atomic-scale technology.

In this talk, recent STM results concerning molecular wires and molecular logic gates will be presented, where on-surface synthesis is applied to investigate the electronic properties of designed molecular systems.

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

Alexander Strobel<sup>1,2</sup>, Filip Kilibarda<sup>1,2</sup>, Elke Scheer<sup>2</sup>, Artur Erbe<sup>1,2</sup>

<sup>1</sup> Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany,

<sup>2</sup> University of Konstanz, Faculty of Sciences, 78457 Konstanz, Germany

Corresponding author: [a.strobel@hzdr.de](mailto:a.strobel@hzdr.de)

Current industrial semiconductor 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 0D molecular systems. This approach offers not only reduction in power consumption and costs, but also a deeper understanding of the electron transport behavior of molecules. Our research focuses on classifying different molecules with the help of Mechanically Controlled Break Junction (MCBJ) technique.

Here we report electrical transport properties of C<sub>60</sub> Fullerene molecules using a unique MCBJ setup. Fullerenes with their high stability and symmetry have become reference molecules for the development of measurement routines for molecular electronics applications. The herein used MCBJ setup enables to evaporate C<sub>60</sub> in situ and determine electrical characteristics under high vacuum conditions. Furthermore, low-temperature measurements down to 10 K are possible. From conductance histograms preferred conductance values of single C<sub>60</sub> molecules are deduced. I-V curves, taken at different conductance values, are fitted using the single level model. Differential measurement methods were applied to get a deeper understanding of electron transport mechanisms in the C<sub>60</sub> molecule.

## DNA-Templated Conducting Polymers for Nanoelectronics

J. Zessin<sup>1</sup>, A. Stern<sup>1</sup>, J. Zhu<sup>2</sup>, B. Ding<sup>2</sup>, M. Mertig<sup>3</sup>, D. Porath<sup>1</sup>

johanna.zessin@mail.huji.ac.il

<sup>1</sup>*Institute of Chemistry and The Center for Nanoscience and Nanotechnology, Hebrew University of Jerusalem, Jerusalem 91904, Israel.*

<sup>2</sup>*National Center for Nanoscience and Technology, Beijing 100190, P. R. China.*

<sup>3</sup>*Kurt-Schwabe Institut für Mess- und Sensortechnik e.V. Meinsberg, Waldheim 04736, Germany.*

DNA is an excellent construction material to build sophisticated devices for nanoelectronics due to the variety of binding sites, the nanometer-sized dimensions and the programmable nature of the Watson-Crick base-pairing. The latter has led to the development of the structural DNA nanotechnology, such as DNA origami,<sup>1</sup> which overcame the linear nature of the canonical DNA towards two- and three-dimensional DNA nanostructures. These DNA-based nanostructures can serve as templates to precisely arrange functional hetero-elements into functional nano-devices. So far, mostly metallic nanoparticles and direct metallization have been used to electrically functionalize such DNA templates towards nanoelectronic devices.

We apply intrinsically conducting polymers (CPs) as functional hetero-elements to build up DNA-templated nanoelectronic devices. Due to their  $\pi$ -conjugated backbone, these organic (semi)-conductors can reach levels of metallic conductivity in certain conditions.<sup>2</sup> CPs are structurally related to DNA and thus, superior to their metallic counterparts with regard to their lightweight and mechanical flexibility. Due to their molecular nature, the conduction mechanism of CPs is more complex than in metals and strongly depends on the molecular design and intermolecular interactions. While their electronic functionality as macroscopic thin films has been successfully demonstrated, proving the electronic functionality of nanoscaled DNA-templated CPs still remains challenging.

We investigated two types DNA-templated CP-nanostructures. First, polyaniline (PANI) was directly polymerized on a Y-shaped double-stranded DNA template forming a supramolecular PANI-DNA nanowire.<sup>3</sup> Second, a water-soluble polythiophene was synthesized and then organized into as a polythiophene nanostructure on a two-dimensional DNA origami template.<sup>4</sup> To reliably contact the polymer nanostructures without destroying or contaminating them, we use a combination of stencil lithography and conductive AFM.<sup>5</sup> A stationary gold electrode, which is characterized by an extremely sharp edge, is evaporated atop the CP nanostructure. The conductive tip of the AFM serves as the second, mobile electrode. Thus, individual CP nanostructures are electrically characterized.

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## Backbone Charge Transport in Double Stranded DNA

Roman Zhuravel<sup>1</sup>, Haichao Huang<sup>1</sup>, Georgia Polycarpou<sup>2</sup>, Liat Katrivas<sup>3</sup>, Dvir Rotem<sup>1</sup>, Joseph Sperling<sup>4</sup>, Alexander B. Kotlyar<sup>3</sup>, Spiros S. Skourtis<sup>2</sup>, Juan Carlos Cuevas<sup>5</sup> and Danny Porath<sup>1\*</sup>

<sup>1</sup> Institute of Chemistry and The Center for Nanoscience and Nanotechnology, The Hebrew University of Jerusalem, Edmond J. Safra Campus, Jerusalem 91904, Israel

<sup>2</sup> Department of Physics, University of Cyprus, Nicosia 1678, Cyprus

<sup>3</sup> Department of Biochemistry and Molecular Biology, George S. Wise Faculty of Life Sciences and Center of Nanoscience and Nanotechnology, Tel Aviv University, Ramat Aviv 69978, Israel

<sup>4</sup> Department of Organic Chemistry, Weizmann Institute of Science, Rehovot 76100, Israel

<sup>5</sup> Departamento de Física Teórica de la Materia Condensada and Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, Madrid, 28049, Spain

Corresponding author: danny.porath@mail.huji.ac.il

Understanding charge transport in DNA molecules is a long-standing problem of fundamental importance across disciplines. It also has a great technological interest due to DNA's ability to form versatile and complex programmable structures. Charge transport in DNA-based junctions has been reported using a great variety of setups, but experiments so far have yielded seemingly contradictory results that range from insulating or semiconducting to metallic-like behaviour. As a result, the intrinsic charge transport mechanism in molecular junction setups is not well understood, which is mainly due to the lack of techniques to form reproducible and stable contacts with individual long DNA molecules. Here we report charge transport measurements through single 30 nm long double stranded DNA molecules with an experimental setup that enables to address individual molecules repeatedly and to measure the current-voltage characteristics from 5 K up to room temperature. Strikingly, we observe very high currents of tens of nanoamperes flowing through both homogeneous and non-homogeneous base-pair sequences. The currents are fairly temperature independent in the range of 5-60 K and show a power law decrease with temperature above 60 K, which is reminiscent of charge transport in organic crystals. Moreover, we show that the presence of even a single discontinuity ("nick") in both strands composing the dsDNA leads to complete suppression of the current, suggesting that the backbones mediate the long-distance conduction in dsDNA, contrary to the common wisdom in DNA electronics.

## Your Notes

## **Your Notes**

## NanoNet International Conference 2019, Dresden

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updated: 05.10.2019 (PZ)

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2) Please, remove your poster on Friday at latest 12:00.

# Self-Organization and Encapsulation of Functional Materials by Peptide Membranes

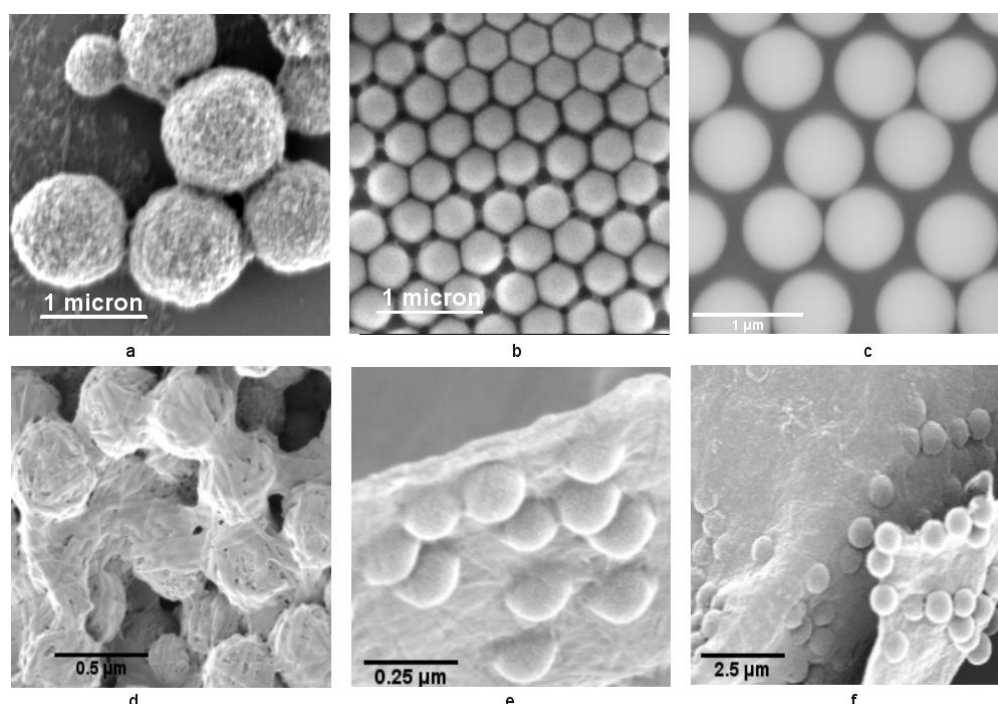
S. Banerjee<sup>1,2,3</sup>, H.-G. Braun<sup>1,2</sup>

<sup>1</sup>IPF Dresden, Dresden, Germany; <sup>2</sup> TU Dresden, Dresden, Germany; <sup>3</sup>Govt. College of Eng. and Ceramic Technology, Kolkata, India

Corresponding author: [semanti26@gmail.com](mailto:semanti26@gmail.com)

Self-organization of peptides such as diphenylalanine (FmocFF) amino acids can be a potent approach to achieve supramolecular fibrils or ribbons assembling into extended membrane(s). By acidification in the bulk, fibrils assemble into 3D hydrogel but pH change at the interface, the growth of the 2D mesh can be achieved which is our area of interest. In association of various colloidal particles having certain functionality, the membrane/sheets or fibrils formed successfully encapsulates the colloids into the mesh and forms well integrated composites. The colloids selected for this purpose was Silica particles of different sizes as well as magnetic materials (Magnetite) of size around 600nm.

This process can be further extended to integrate other colloids contributing various functionality or specificity to the composites synthesized from surface bound biomaterials. The use of magnetic materials is especially important for its affinity to bio-membrane and its ability for drug transport to target as well as concentration of particle entrapped.



a: Magnetite particles, b: Colloidal Silica (180-200nm), c: Colloidal Silica (600-800nm) entrapped in the membrane shown d, e and f respectively.

# A platform for quantitative analysis of biochemical processes in droplets using nano-sensors.

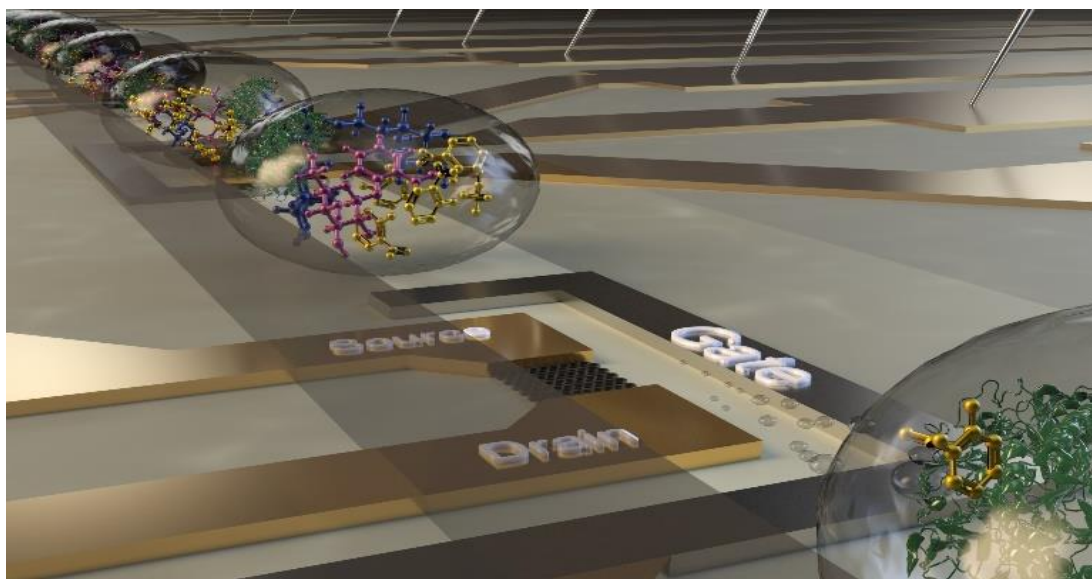
Dmitry Belyaev,<sup>a</sup> Julian Schütt,<sup>a</sup> Larysa Baraban,<sup>a,b</sup> Gianaurelio Cuniberti<sup>a,b</sup>

<sup>a</sup> Max Bergmann Center of Biomaterials and Institute for Materials Science, Dresden University of Technology, Budapesterstrasse 27, 01069 Dresden, Germany

<sup>b</sup> Technische Universität Dresden, Center for Advancing Electronics Dresden, 01062, Dresden, Germany

dmitry.belyaev@tu-dresden.de

Real-time monitoring of bio-chemical processes, e.g. related to cancer development and treatment is high societal relevance. This can be done by implementing miniaturized lab-on-a-chip detecting systems, incorporating microfluidics and Si nanowire field-effect transistor (SiNW FET) chip allowing droplet analysis<sup>[1]</sup>. Here, the chemical reaction of  $\beta$ -galactosidase ( $\beta$ -gal) and ortho-nitrophenol-galactose (ONPG) was detected in a label-free format, and the kinetics was analyzed using SiNW FET.  $\beta$ -gal is an essential enzyme in the human body which drives glycolysis by hydrolyzing lactose. SiNW FET is an ion-sensitive device and it is able to detect the presence of charged molecules or ions in the liquid environment. The reaction was analyzed in numerous emulsion droplets generated in a microfluidic flow-cell, by means of honeycomb-shaped NW FET chip. The flow cell was produced via combination of laser, UV and soft lithography techniques and consists of the droplets generation module and the channel structure with width of about 300  $\mu\text{m}$ , and is successfully integrated on silicon chip. We attribute the shift of the  $I_{\text{sd}}$  current to the change on ionic composition of the media. Statistical analysis of peaks is presented along with the comparison of the data for the assay and the reference. Comparative data proved successful detection of the reaction.



*Fig.1 – Schematic representation of the system for biochemical analysis in droplets, implementing FET sensor and microfluidics channel.*

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## Poster Contribution - Abstract

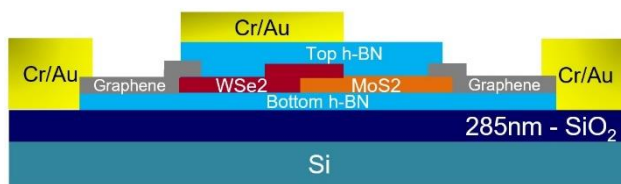
# Band-to-band tunnelling in two-dimensional van der Waals heterostructures.

**Phanish Chava**, Vivek Koladi, Himani Arora, Manfred Helm, Artur Erbe

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

Email : [p.chava@hzdr.de](mailto:p.chava@hzdr.de)

Quantum mechanical band-to-band tunneling (BTBT) is a particular type of carrier injection mechanism, which is responsible for the electronic transport in tunneling based devices like Esaki diode and Tunnel Field Effect Transistor (TFET). Atomically thin layers of transition metal dichalcogenides (TMDCs) are promising semiconducting materials for realizing such devices owing to their sharp interfaces. We demonstrate BTBT between the layers of molybdenum disulfide (MoS<sub>2</sub>) and tungsten diselenide (WSe<sub>2</sub>) in a MoS<sub>2</sub>-WSe<sub>2</sub> heterojunction, encapsulated with hexagonal boron nitride (h-BN) on the top and bottom. In addition, we employ few-layer graphene as the contact material to the heterojunction thereby forming a 2D-2D van der Waals contact. We observe negative transconductance and negative differential resistance in the fabricated device thereby indicating the tunnelling behaviour.





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

Kristina Ditte<sup>1,2</sup>, Dr. Franziska Lissel<sup>1,2</sup>, Dr. Anton Kiriya<sup>1</sup>, Prof. Brigitte Voit<sup>1,2</sup>

<sup>1</sup>Leibniz-Institut für Polymerforschung 01069 Dresden, Germany

<sup>2</sup>Technische Universität Dresden Mommsenstraße, 01062 Dresden, Germany

Corresponding author: ditte@ipfdd.de

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 this work 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 is achieved by creating “second order” block copolymers, i.e. by alternating rigid-rod PSC units and PDMS chains with different molecular weights ( $M_w = 1000, 2500$  and  $25000$  g/mol). In the resulting second-order hybrids, the two components are compartmentalized 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. X-Ray analysis and TEM imaging were performed to ensure a phase separation of these two components. Additionally, transistor characteristics and charge carrier mobilities were analyzed by fabricating bottom-contact devices and compared with the reference pure DPP polymer.

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# Ion beam implanted Germanium nanowires

Ahmad Echresh<sup>a,b</sup>, Yufang Xie<sup>a</sup>, Slawomir Prucnal<sup>a</sup>, Lars Rebohle<sup>a</sup>,  
Yordan M. Georgiev<sup>a,c</sup>

<sup>a</sup> Institute of Ion Beam Physics and Materials Research, HZDR, Dresden, 01328, Germany

<sup>b</sup> International Helmholtz Research School for Nanoelectronic Network, HZDR, Dresden,  
01328, Germany

<sup>c</sup> On leave of absence from the Institute of Electronics at Bulgarian Academy of Sciences, 72,  
Tsarigradsko chausse blvd., Sofia, 1784, Bulgaria  
e-mail: [a.echresh@hzdr.de](mailto:a.echresh@hzdr.de)

Keywords: Ion beam implantation; Flash lamp annealing; Doping; p-n junction; Infrared sensor

Germanium (Ge) is a promising high mobility channel material for future nanoelectronics. 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 [1].

The introduction of impurity atoms allows the tuning of the electrical properties of the semiconductor material. Ion beam implantation is an industrial standard for semiconductor's doping as it can incorporate single ion species with a single energy in a highly controlled fashion. However, the destructive nature of ion beam implantation requires a crystal recovery step such as an annealing process [2].

In this work, Germanium-on-insulator (GeOI) substrates were doped with phosphorous (P) using ion beam implantation followed by flash lamp annealing (FLA). During FLA process the implanted layer recrystallized and P was electrically activated. Then Ge nanowires were fabricated using electron beam lithography (EBL) and inductively coupled plasma (ICP) etching. Raman spectra showed the amorphisation of Ge structure after implantation and good recovery after FLA (Fig. 1). Rutherford backscattering spectrometry (RBS) measurements in random (R) and channeling (C) modes (Fig. 2) were used to verify the crystal quality of Ge layer before and after FLA. As one can see, the yield intensity of the channeling mode was increased after implantation, which can be related to amorphisation of the top Ge layer. Also, the yield peak of flashed GeOI has a good match with unimplanted counterpart, which shows the good recrystallization during FLA. Moreover, we designed Hall effect measurement configuration for single Ge nanowires (Fig. 3) to determine the carrier mobility and carrier concentration. The results of these measurements will be shown at the conference [3,4]. The goal is to fabricate p-n junction along the Ge nanowires and use it as an infrared sensor.

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# Comprehensive study on the device performance of ultra-scaled CNTFETs

Florian Fuchs<sup>1,2,4</sup>, Anibal Pacheco-Sanchez<sup>5</sup>, Andreas Zienert<sup>1,2</sup>, Sven Mothes<sup>4,5</sup>,  
Martin Claus<sup>4,5</sup>, Sibylle Gemming<sup>1,3,4</sup>, and Jörg Schuster<sup>1,2,4</sup>

<sup>1</sup>Chemnitz University of Technology, Chemnitz, Germany

<sup>2</sup>Fraunhofer Institute for Electronic Nano Systems, Chemnitz, Germany

<sup>3</sup>Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

<sup>4</sup>Center for Advancing Electronics Dresden, Dresden, Germany

<sup>5</sup>TU Dresden, Dresden, Germany

Corresponding author: florian.fuchs@enas.fraunhofer.de

We study ultra-scaled carbon nanotube based field-effect transistors (CNTFETs) with channel lengths down to 5.1 nm. Computationally expensive atomistic quantum transport simulation (AQS) as well as numerical device simulations (NDS) are employed (Pacheco-Sanchez et al., IEEE TNANO 17, 100, 2018).

The NDS approach is critically tested and verified by comparing the results with the more expensive AQS approach. A simplified device with ohmic-like contacts is studied for this purpose, consisting of a (16,0) CNT. We demonstrate that tunneling processes in the transistor are adequately described by the NDS approach and discuss deviations, which we attribute to a different description of the contact physics.

Having verified the NDS, we apply it to compare different device architectures with Schottky contacts, including gate-all-around, buried gate, and top-gate designs. Different figures of merits such as the subthreshold slope and the  $I_{on}/I_{off}$  ratio are compared. It is shown that the buried gate CNTFET is the most suitable structure for high performance logic applications. Also the benefits of having doped spacer regions are demonstrated. Structural changes such as displaced gates are also studied towards improving the device performance.

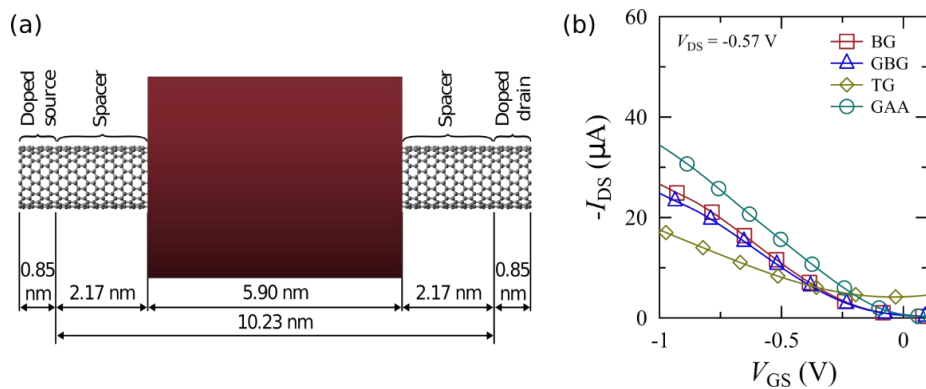


Fig. 1: (a) Exemplary device structure used in AQS. The contacts are n-doped, yielding ohmic-like contacts. (b) Device characteristics for CNTFETs with Schottky contacts and with different gate architectures.

# Fabrication and Electrical Characterization of Top Gated RFETs

Sayantan Ghosh<sup>1</sup>, Muhammad Bilal Khan<sup>1</sup>, Dr. Artur Erbe<sup>1</sup>, Dr. Yordan M. Georgiev<sup>1,2</sup>

<sup>1</sup>Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Bautzner Landstr. 400, 01328 Dresden, Germany

<sup>2</sup>Institute of Electronics at Bulgarian Academy of Sciences, 72, Tsarigradsko Chausse Blvd., 1784 Sofia, Bulgaria

Corresponding author: [s.ghosh@hzdr.de](mailto:s.ghosh@hzdr.de)

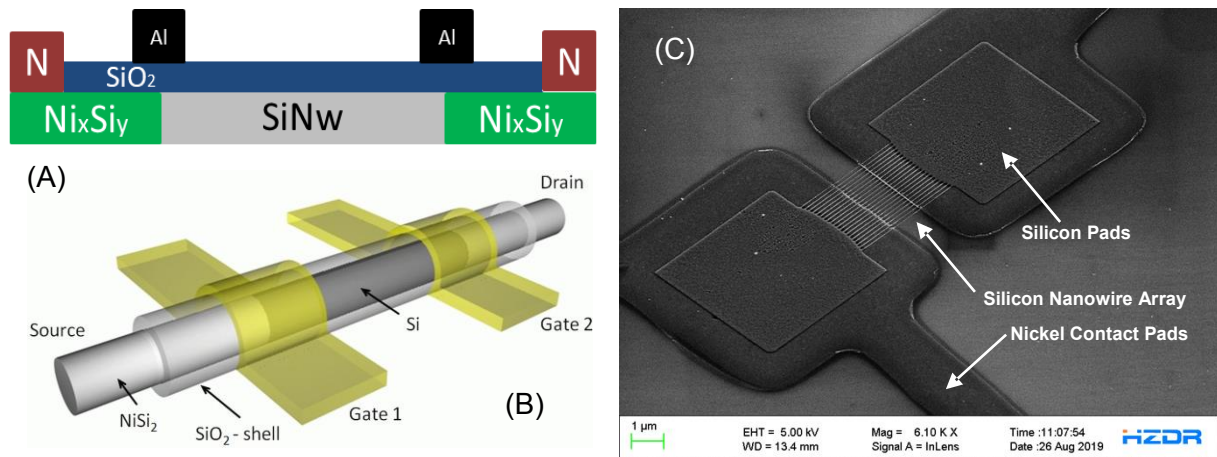


Figure: (A) Cross section of two top gated RFETs; (B) Overall schematic of RFET [1]; (C) SEM image of Silicon nanowire array with Nickel contacts

Following Moore's Law, the concept of "*Beyond CMOS*" came into picture which incorporated emerging new research and technology. One such concept which presents the idea of a universal transistor to replace CMOS in the near future is called the Reconfigurable Field Effect Transistors (RFET). RFETs can be dynamically programmed to p or n polarity by the application of electrostatic potential. In this work, these are silicon nanowire (SiNW) based transistors with two gates. One of the gates known as the "Program Gate" is used to tune the device polarity, while the other gate known as the "Control Gate" modulates the flow of charge carriers. For the fabrication of the devices, nickel is placed at both the ends of the nanowire and subsequently annealing is performed. This results in the formation of NiSi<sub>2</sub>-Si-NiSi<sub>2</sub> Schottky junctions and such devices show ambipolar behavior when controlled by a back gate or single top gate. For unipolar behavior, two top gates are fabricated on top of the two Schottky junctions. Flash Lamp Annealing (FLA) is used for silicidation of NWs instead of Rapid Thermal Annealing (RTA) as the former yields a significantly better control over the silicidation process.

This work aims at the top down fabrication of silicon nanowires followed by optimization of oxide shell/gate dielectric around it. Various material combinations are tried to create the gate dielectric for better control over the conduction of charge carriers. At the end, the top gates and drain/source contacts are fabricated followed by electrical characterization of the devices. These novel reconfigurable nanowire transistor devices are capable of carrying out flexible logic operations during their performance. Their simple and compressed architecture can be used for future circuit designs yielding complimentary logic functions.

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## **Dry-electrical functionalization of monolayer graphene and its electric investigation**

Benjamin Hacker<sup>1</sup>, Daniela Dasler<sup>2</sup>, Frank Hauke<sup>2</sup>, Andreas Hirsch<sup>2</sup>, Vojislav Krstić<sup>1</sup>

<sup>1</sup>Departement of Physics, FAU, Erlangen, Germany

<sup>2</sup>Departement of Chemistry, FAU, Erlangen, Germany

Corresponding author: [benjamin.hacker@fau.de](mailto:benjamin.hacker@fau.de)

The modification of graphene is of high interest, since it offers many possibilities to change and control its electronic properties. A way to achieve this is covalent functionalization, which requires a local conversion of  $sp^2$ - to  $sp^3$ -bonds. A large group of molecules, which are of interest for this experiment, have to be provided with additional electrical charge in order to achieve the conversion. This is often done in solution, which has shown to have certain disadvantages, especially with regard to electrical measurements. Here, a method will be presented, how this process can be done by dry-gating in a highly controlled environment with on-chip integrated individual graphene monolayer devices. A successful functionalization is confirmed via Raman and electrical measurements, which demonstrates the feasibility of the approach.

## Synthesis and characterization of a solution-processable Ru-polymetallayne

Po-Yuen Ho<sup>1</sup>, Hartmut Komber<sup>1</sup>, Evgenia Dmitrieva<sup>2</sup>, Ulrike Kraft<sup>3</sup>, Stefan Mannsfeld<sup>4</sup>,  
Henning Sirringhaus<sup>3</sup> and Franziska Lissel<sup>1,5</sup>

<sup>1</sup>Institute for Macromolecular Chemistry (IMC), Leibniz Institute of Polymer Research Dresden (IPF), Hohe Str. 6, 01069 Dresden, Germany. <sup>2</sup>Leibniz Institute for Solid State and Materials Research (IFW), Helmholtz str. 20, 01069 Dresden. <sup>3</sup>University of Cambridge, Cavendish Laboratory, J J Thomson Avenue, Cambridge, CB3 0HE, United Kingdom. <sup>4</sup>cfaed Center for Advancing Electronics Dresden, Technical University Dresden, 01062 Dresden. <sup>5</sup>Faculty of Chemistry, Technical University Dresden, 01062 Dresden.

Corresponding author: [lissel@ipfdd.de](mailto:lissel@ipfdd.de), [ho@ipfdd.de](mailto:ho@ipfdd.de)

Metallopolymers are of great interest due to their unique properties compared to their pure organic counterparts, i.e. enhanced spin-orbit coupling and high redox activity etc<sup>1</sup>. Among these, polymetallaynes, in which the metal center is integral part of the conjugated backbone, have attracted immense interest due to their unique charge physical properties<sup>2</sup> and potential for electronic applications such as organic field effect transistors (OFET) or organic photovoltaics (OPV)<sup>3</sup>. However, the vast majority of functional polymetallaynes are Pt-/Pd-containing<sup>1</sup>, which are not redox-active. To achieve high redox activity, other transition metals such as group 8 metals can be used. Yet, the main problem of it is the lack of synthetic pathway to this class of redox-functional group 8-based polymetallaynes and we herein report the successful synthesis of a Ru-based polymetallayne with various characterizations.

In this study, inspired by the work of Touchard et al. and Akita et al.<sup>2,4</sup>, the synthetic method of dehydrohalogenation is successfully transferred to polymerization and a novel Ru(II) containing polymetallayne realized. The polymer is solution-processable and was investigated by various methods, ranging from structural characterizations such as NMR to electrical characterization. The redox-active behavior of the metal center is retained, and semiconducting behavior of the polymer is observed. The presented work details a new synthetic pathway to functional polymetallaynes and demonstrates the promise of Ru-polymetallayne for electronic applications.

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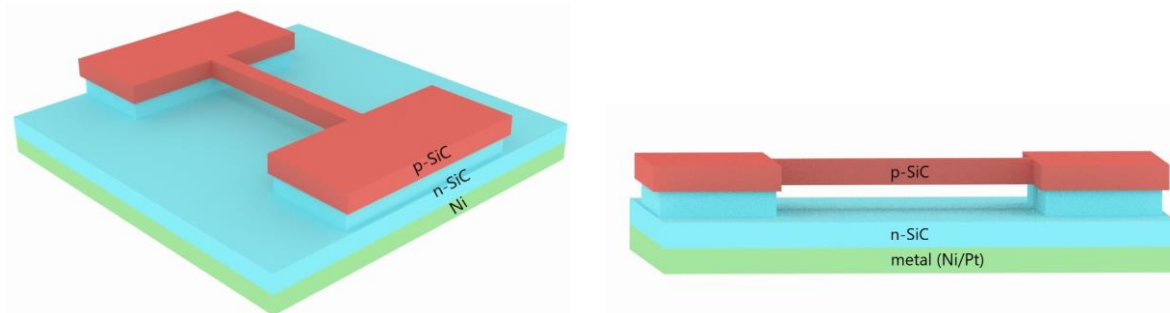
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# Fabrication and Characterization of string resonators in silicon carbide for Hybrid Spin-Mechanical systems

Nagesh S. Jagtap<sup>1</sup>, Artur Erbe<sup>1</sup>, Yordan M. Georgiev<sup>1</sup>, Georgy Astakhov<sup>1</sup>

<sup>1</sup>Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

Corresponding author: [n.jagtap@hzdr.de](mailto:n.jagtap@hzdr.de)



## Abstract:

Microelectromechanical systems are miniaturized lab-on-a-chip systems widely used for sensing and actuation. Their applications can be found in various fields such as automotive, consumer electronics, defense, aeronautics, medical and communication systems.

Wide band-gap (2.3-3.3 eV) semiconductors such as silicon carbide (SiC) are especially important for harsh environment and power electronics applications due to high breakdown field. Some of the point defects in SiC can act as color centers and can potentially be used for bioimaging, nanosensing, magnetic field and temperature sensing. Color centers carrying a net electron spin are useful for spin manipulation techniques: Electron Paramagnetic Resonance (EPR) and Optically Detected Magnetic Resonance (ODMR). It shows that they are potential candidate for quantum metrology, quantum computing and spintronics.

Hybrid spin-mechanical systems are promising for quantum technologies. Spin-mechanical resonance is observed when a spin resonance frequency matches a resonance frequency of a mechanical mode and it reduces the spin relaxation time owing to resonantly enhanced spin-phonon coupling. SiC is a better candidate than diamond for such hybrid systems because of highly coherent spin centers. Some possible applications have been theoretically proposed: low-temperature ODSMR magnetometry, accelerometry, small magnetic field and mass sensing, spin-mediated cooling and heating of mechanical modes. The main focus of the project is to practically realize ODSMR magnetometry and to determine the change in resonant frequency after implanting defects.

In this work, design is transferred using Electron Beam Lithography. Inductively Coupled Plasma – Reactive Ion Etching is used to etch the material anisotropically. Then dopant selective photoelectrochemical etching will be used to under etch n-SiC and release resonator structures of p-SiC. Characterization will be done using piezoelectric and optical detection method.



# Synthesis of nickel nanoparticles using DNA Origami molds

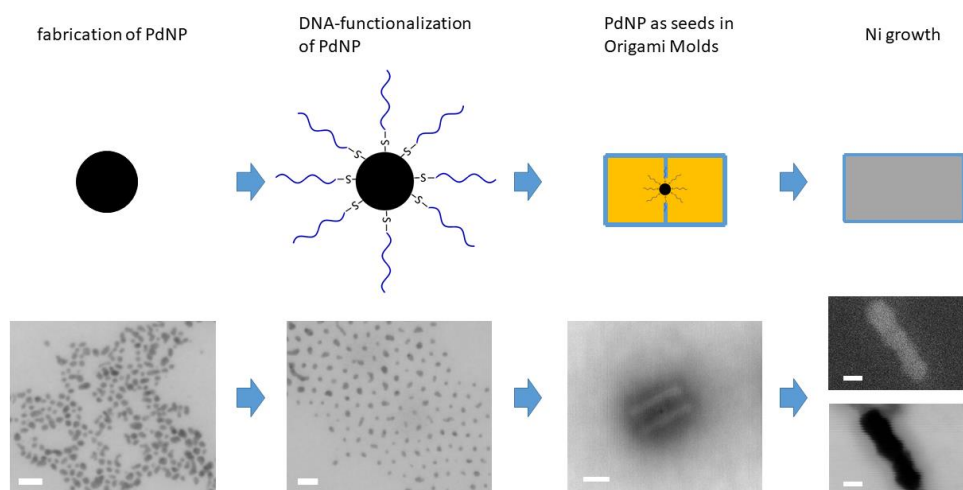
Ulrich Kemper<sup>1</sup>, Jingjing Ye<sup>1</sup>, Ralf Seidel<sup>1</sup>

<sup>1</sup>Peter Debye Institute for Soft Matter Physics, Universität Leipzig, Germany

Corresponding author: ralf.seidel@physik.uni-leipzig.de

A challenge for the bottom-up fabrication of nanoelectronic devices is the accurate material deposition on the nanometer scale. Concerning biomolecular materials, DNA nanotechnology meets this challenge by being highly precise at building DNA structures of nearly any desired form. We recently introduced the concept of a DNA origami mold-based particle synthesis that allows the synthesis of inorganic nanoparticles with programmable shape. Particularly, we demonstrated the fabrication of 40 nm long rod-like gold particles with quadratic cross-section [1] as uniform micrometer-long conductive gold nanowires of 20-30 nm diameter [2]. Direct conductance measurements demonstrated the metallic conductivity of these wires.

Here, we expand the mold-based fabrication method to nickel, being a ferromagnetic material. To allow a seeded-growth of nickel inside the origami molds, palladium nucleation centers needed to be introduced into the mold cavity. We therefore synthesized palladium nanoparticles and established an efficient functionalization protocol of the particles with single-stranded DNA. The functionalized particles were bound to complementary DNA strands inside the mold cavity from which a seeded nickel deposition was initiated. This provided rod-like nickel nanoparticles with an average diameter of 25 nm. The introduction of magnetic domains in the mold-based fabrication scheme provides a possible route to establish nanoscopic spin-valve structures.



**Figure 1.** Scheme and tSEM images illustrating the mold-based synthesis procedure of nickel nanostructures. Palladium nanoparticles were synthesized, functionalized with single stranded DNA and placed inside DNA origami molds. These particles were used as a nucleation center for a seeded nickel growth while the origami shell confined the resulting structure. Scale bar: 20nm.

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# Segmentation and classification of molecular IV data

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

<sup>1</sup>Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

<sup>2</sup>Centre for DNA Nanotechnology department of Chemistry and Interdisciplinary Nanoscience Center, 8000 Aarhus C, Denmark

Current industrial scaling processes are reaching limits. We see not only diminishing 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 two different kinds of measurements. One is performed in a liquid solution and under ambient conditions, and the other one in a cryogenic environment, under vacuum. As a testbed for these measurements, we use salen and C60 molecules respectively.

We show how this data fits to the basic Single Level Model and what are the possible pitfalls of this approach. As an alternative, we offer modified versions of the SLM and compare them at predicting the transport properties of the molecules.

Furthermore, due to the inherently stochastic processes of molecular binding to the nanoscopic junction, we propose an efficient approach based on the Machine Learning to further cluster the data into subsets. By using auto-encoders and decision trees with minimal amounts of supervised learning we can cluster large quantities of data.

This allows us to evaluate different binding positions and events, with most appropriate models, and extract the underlying data.

# Multiplexed detection of stress hormone cortisol in saliva using silicon nanowire field effect transistors with a portable measurement system

S. Klinghammer<sup>1</sup>, N. Licciardello<sup>1</sup>, T. Voitsekhivska<sup>2</sup>, C. Kirschbaum<sup>3</sup>, L. Baraban<sup>1</sup>, G. Cuniberti<sup>1</sup>

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

<sup>2</sup>Helmholtz-Zentrum Dresden-Rossendorf e.V., Institute of Ion Beam Physics and Materials Research, 01328 Dresden, Germany

<sup>3</sup>Department of Psychology, TU Dresden, 01062 Dresden, Germany

Corresponding author: Stephanie.Klinghammer@nano.tu-dresden.de

The accurate and rapid biomolecular detection of numerous samples from multiple patients on portable point-of-care devices is attracting great attention in bio- and nanotechnology for more than a decade [1]. Here, we demonstrate a portable, multiplexed, label-free and real-time sensing platform for detection of small molecules based on silicon nanowire field effect transistors [2]. We particularly focus on the sensitive recognition of the stress hormone cortisol by using aptamers as receptors in order to allow high sensitive screenings in more physiological conditions. Figure 1 shows structure and electrical response of an individual FET upon cortisol injection of different concentrations. Finally, we show the working principle. Determination of cortisol levels in saliva of volunteers are detected and compared to those obtained with conventional ELISA method.

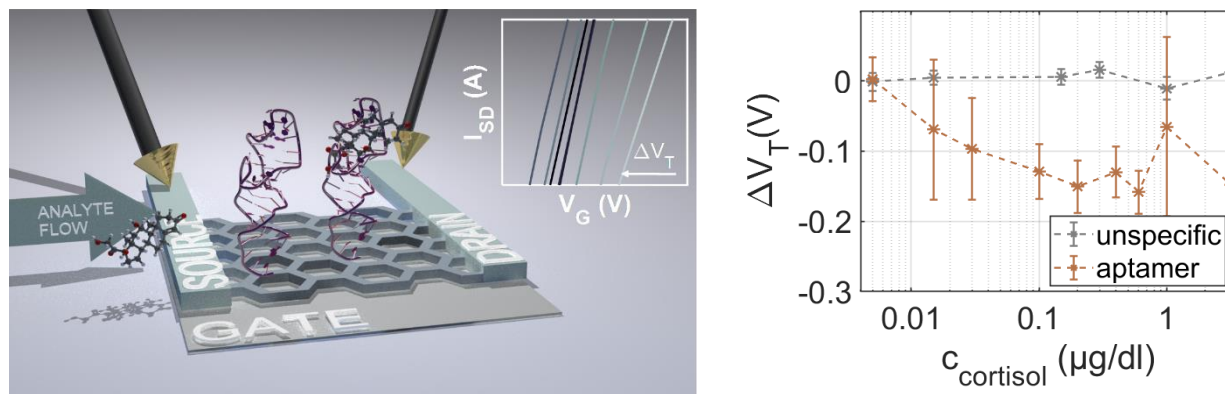


Figure 1: Left: Schematic drawing of honeycomb structured FET. Inset: Shift of transfer curve upon injection of target cortisol at various concentrations. Right: Shift of threshold voltage in dependence on target concentration.

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# Transmitting rotation between molecular gears on Au(111)

Tim Kühne,<sup>1,2</sup> Kwan Ho Au Yeung,<sup>1,2</sup> Gianaurelio Cuniberti,<sup>1,2,3</sup> and

*Francesca Moresco*<sup>1,2</sup>

<sup>1</sup>Institute for Materials Science, TU Dresden, 01062 Dresden, Germany

<sup>2</sup>Center for Advancing Electronics Dresden, TU Dresden, 01062 Dresden, Germany

<sup>3</sup>Dresden Center for Computational Materials Science (DCMS), TU Dresden, 01062 Dresden, Germany.

Corresponding author: tim.kuehne@tu-dresden.de

A fundamental component of a planar single-molecule mechanical machine is a molecular gear, whose construction needs a proper combination of the molecular design, a smart selected surface for anchoring as well as the controlled rotation by manipulation. We investigated the adsorption of pentaphenylcyclopentadiene molecules (PPCP) and derivatives on Au(111) by LT-STM. Both pristine and radical state of the molecules after tip-induced cleaving at the cyclopentadiene core have been studied. The step-by-step rotation and transmission of rotation has been examined using the lateral manipulation mode of the STM.

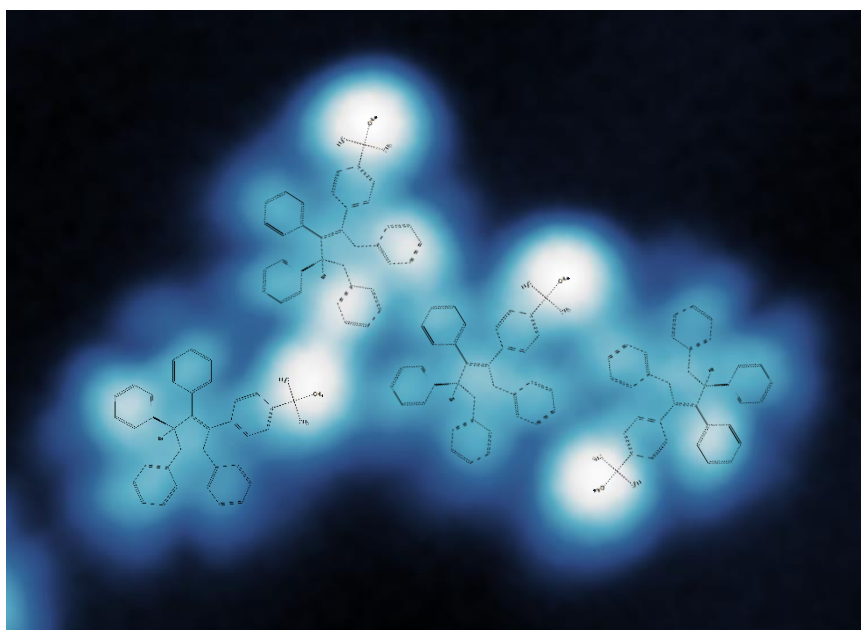


Fig. 1 PPCP molecules containing a tert-Butyl group on Au(111). The molecules are positioned like a train of gears, ready in a position for rotation. Image size 5.5 x 4 nm<sup>2</sup>, taken at bias 1 V and current 2 pA.

## Molecular chain formation at surfaces: PEEB/Au(111) - A High-throughput Study

Lokamani<sup>1,2</sup>, Jeffrey Kelling<sup>3</sup>, Jörg Meyer<sup>1</sup>, Anja Nickel<sup>1</sup>, Robin Ohmann<sup>1</sup>, Gianaurelio Cuniberti<sup>1,4</sup>, Jannic Wolf<sup>5</sup>, Thomas Huhn<sup>5</sup>, Peter Zahn<sup>2</sup>, Francesca Moresco<sup>1</sup> and Sibylle Gemming<sup>2,6</sup>

1 Institute for Materials Science and Max Bergmann Center of Biomaterials,  
Technische Universität Dresden, Dresden, Germany

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

3 Department of Information Services and Computing, HZDR, Dresden, Germany

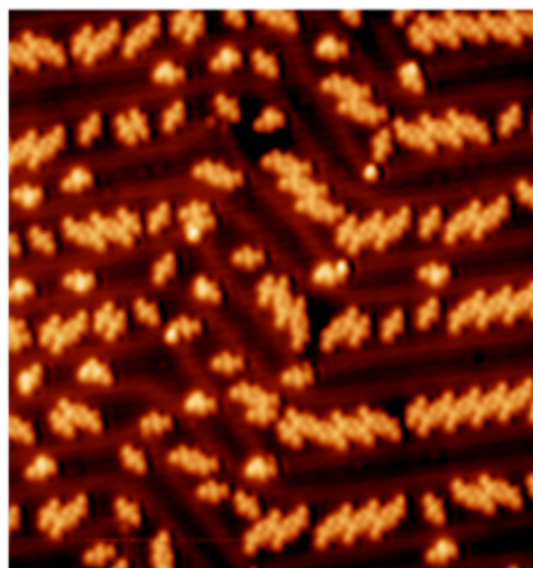
4 Division of IT Convergence Engineering, POSTECH, Pohang, Republic Korea

5 Department of Chemistry, Universität Konstanz, Konstanz, Germany

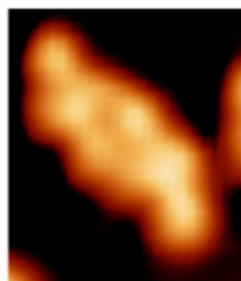
6 Institute of Physics, Technische Universität Chemnitz, Chemnitz, Germany

Corresponding author: m.lokamani@hzdr.de

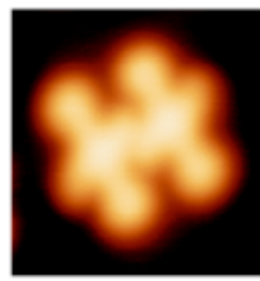
The electronic and geometrical structure of PEEB molecules adsorbed on the Au(111) surface is investigated by low temperature STM and STS in conjunction with DFTB simulations of the density of states, of the interaction with the substrate and of the intermolecular interactions. Our DFT calculations indicate that the PEEB molecule is physisorbed on the Au(111) substrate, with negligible distortion of the molecular geometry and charge transfer between the molecule and the substrate. Additionally, due to the low corrugation of the Au(111) surface, PEEB molecules can form quasi interlocked lateral patterns, which are observed in STM experiments. In order to explain the interlocked lateral patterns, we employ DFTB+ based high-throughput calculations including universal force field for dispersion corrections to evaluate an energy function, which incorporates the adsorption energy of single PEEB molecules on the metal surface and the intermolecular interaction energy of a pair of PEEB molecules. The analysis of the energy function reveals, that depending on coverage density specific types of pattern are preferred and can be exploited to form one-dimensional molecular wires on Au(111).



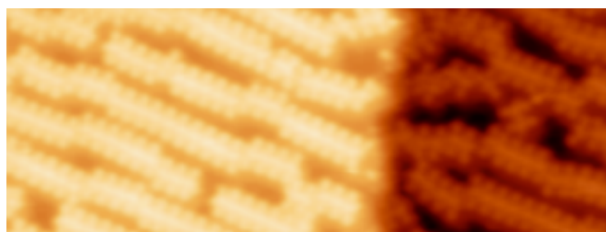
(a) STM (39 X 39 nm<sup>2</sup>)



(b) Hunter's fence



(c) Normal fence



(d) Mono-layer

# Raman study of Ag–In–S quantum dots obtained from aqueous solutions in the presence of glutathione or mercaptoacetic acid

B.V. Lopushanska<sup>1</sup>, Y.M. Azhniuk<sup>1,2</sup>, Sh.B. Molnar<sup>1</sup>, O. Selyshchev<sup>3</sup>,  
V.V. Lopushansky<sup>2</sup>, I.P. Studenyak<sup>1</sup>, D.R.T. Zahn<sup>3</sup>

<sup>1</sup> Uzhhorod National University, Uzhhorod, Ukraine

<sup>2</sup> Institute of Electron Physics, Ukr. Nat. Acad. Sci., Uzhhorod, Ukraine

<sup>3</sup> Semiconductor Physics, Chemnitz University of Technology, Chemnitz, Germany

Corresponding author: lopushanska5@gmail.com

Ag–In–S water-soluble colloidal quantum dots (QDs) are known for their intense luminescence. They are composition- and size-tunable across the whole visible spectral range and are promising for applications as light sources, solar cells, in photocatalysis and biology [1, 2]. Here we report on the synthesis and optical characterization of size-selected non-stoichiometric Ag–In–S QDs and Ag–In–S/ZnS core/shell nanoparticles synthesized from AgNO<sub>3</sub>, InCl<sub>3</sub>, and Na<sub>2</sub>S aqueous solutions in the presence of glutathione (GSH) or mercaptoacetic acid (MAA). Zinc acetate was added at the second stage of the reaction to form ZnS shell on the QDs. The nanoparticle size selection was performed by repeated fractioning of the colloidal solutions by precipitation at 4000 rpm in the presence of a non-solvent (2-propanol).

The colloidal solutions of the Ag–In–S and Ag–In–S/ZnS QDs were characterized by optical absorption (Cary 50), photoluminescence (Shimadzu RF-6000), and Raman (LabRAM,  $\lambda_{\text{exc}} = 325, 488, \text{ and } 515 \text{ nm}$ ) spectroscopies. The optical absorption edge and photoluminescence maxima exhibit a clear size-dependent shift. Band gap values were determined from Tauc plots (for direct allowed optical transitions). The average QD size was estimated from the correlation between the band gap and the QD size based on optical absorption and TEM data [1]. The value of the Stokes shift increases with decreasing QD size from 0.14 eV (for 3.2 nm QDs) to 0.48 eV (for below 2 nm QDs)..

We observed more features in the Raman spectra than in earlier studies of nonstoichiometric Ag–In–S QDs [1, 2] and assigned the Raman peaks to the corresponding bond vibrations. Raman spectra of zinc acetate-treated samples measured at resonance excitation (325 nm) show typical ZnS LO and 2LO phonon peaks, contrary to the off-resonance spectra of the same samples measured at 488 nm. This can be an evidence for the ZnS shell formation.

On the other hand, the optical absorption spectra of Ag–In–S/GSH QDs indicate that the addition of Zn at the second stage of the QD fabrication process results rather in the formation of Zn-doped Ag–In–S QDs than Ag–In–S/ZnS nanostructures. Details related to the ZnS shell formation and/or Zn introduction in the Ag–In–S QDs as well as effects of  $[\text{Ag}^+]:[\text{In}^{3+}]:[\text{S}^{2-}]$  component ratio on the optical properties of the QDs formed require additional studies.

[1] A. Raevskaya, V. Lesnyak, D. Haubold, V. Dzhagan, O. Stroyuk, N. Gaponik, D.R.T. Zahn, A. Eychemüller, J. Phys. Chem. C 2017, 121, 9032–9042.

[2] O. Stroyuk, A. Raevskaya, F. Spranger, O. Selyshchev, V. Dzhagan, S. Schulze, D.R.T. Zahn, A. Eychemüller, J. Phys. Chem. C 2018, 122, 13648–13658.

## **Gating technologies for bilayer 2D carrier systems**

Jana M. Meyer<sup>1</sup>, J. Scharnetzky<sup>2</sup>, M. Berl<sup>2</sup>, S. Parolo<sup>2</sup>, W. Wegscheider<sup>2</sup>, M. Hauser<sup>3</sup>,  
W. Dietsche<sup>2,3</sup>, L. Tiemann<sup>1</sup> and R. H. Blick<sup>1</sup>

<sup>1</sup>Center for Hybrid Nanostructures, University of Hamburg, 22761, Germany

<sup>2</sup>ETH Zürich, 8092 Zürich, Switzerland

<sup>3</sup>Max-Planck-Institute for Solid State Research, 70569 Stuttgart, Germany

Corresponding author: [jameyer@physnet.uni-hamburg.de](mailto:jameyer@physnet.uni-hamburg.de)

In nanotechnology, electrostatic gating of two-dimensional carrier systems is crucial to change the intrinsic electron density, that is given by doping in the growth process. In bilayer systems such as gallium arsenide double quantum wells, electrical separation of the two layers and independent control of the carrier densities can be achieved with a complex system of structured back gates and metallic top gates. The back gates are patterned previous to the overgrowth with the double layer system. This technology is a versatile tool to generate confinement potentials, tune the carrier concentration and study a variety of quantum phenomena.

# Naphthalene Diimide Ammonium Based Perovskite Like Crystal Complexes

Goutham Raj Perumallapelli<sup>1#§</sup>, Anton Kiri<sup>1#\*</sup> and Brigitte Voit<sup>1§\*</sup>

<sup>1</sup>The Leibniz Institute of Polymer Research Dresden (IPF), Germany.

<sup>#</sup>IHRS Nanonet, HZDR, Rossendorf, Dresden, Germany.

<sup>§</sup>The Technische Universität Dresden, Germany.

\*Corresponding authors

Corresponding author: [kiri@ipfdd.de](mailto:kiri@ipfdd.de) , [Voit@ipfdd.de](mailto:Voit@ipfdd.de)

Two-dimensional (2D) semiconductors featuring sizable bandgaps and strong in-plane charge transport have opened up new opportunities for nano-electronics and optoelectronics.<sup>1,2</sup> Organic-inorganic halide perovskites (OIHPs) are particularly attractive, which combine the excellent carrier transport inherent to the inorganic semiconductors together with the processability and flexibility of the organic semiconductors, therefore are ideal for wafer-scale fabrication of flexible electronic and optoelectronic devices by bottom-up approaches. Naphthalene diimide (NDI) is very well known-type semiconductor material, which has been studied very well in organic field effect transistors. Typically, the conventional perovskites have simple aliphatic or aromatic molecules as organic cation. Whereas, NDI ammonium iodide is a very bulky molecule. We have characterized the NDI based perovskite like complexes (NDI + PbI<sub>2</sub>) using various characterization techniques in order to confirm the formation of the complex.

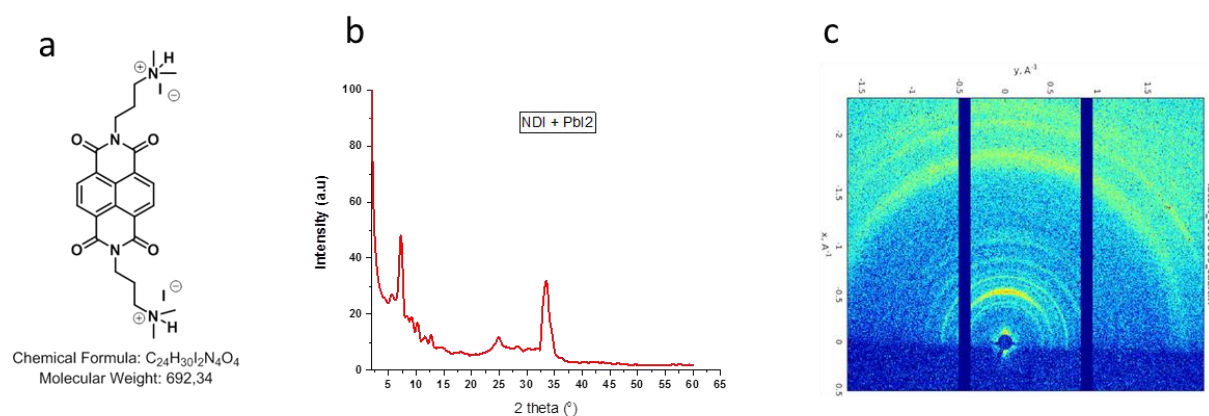


Figure 1 : (a) Chemical structure of NDI ammonium iodide molecule, (b) X-Ray Diffraction pattern of the perovskite like complex, (c) 2D GIWAXS for NDI + PbI<sub>2</sub> mixture

## References:

1. Wang, Q.; Kalantar-Zadeh, K.; Kis, A.; Coleman, J. N.; Strano, M. S. *Nat. Nanotechnol.* 2012, 7, 699–712.
2. Zeng, M.; Xiao, Y.; Liu, J.; Yang, K.; Fu, L.; *Chem. Rev.* 2018, 118, 6236–6296.

## Ab-initio study on morphology of donor-acceptor polymers

F. Günther<sup>1,2</sup>, K. Preis<sup>3</sup>, A. Rehn<sup>1</sup>; Lokamani<sup>1</sup>; P. Zahn<sup>1</sup>, S. Gemming<sup>1,3</sup>

<sup>1</sup> Institute of Ion Beam Physics and Materials Research, HZDR, 01328 Dresden, Germany

<sup>2</sup> Faculty of Chemistry, TU Dresden, 01062 Dresden, Germany

<sup>3</sup> Institute of Physics, TU Chemnitz, 09107 Chemnitz, Germany

Corresponding author: [florian.guenther@chemie.tu-dresden.de](mailto:florian.guenther@chemie.tu-dresden.de)

Donor-acceptor (DA) polymers have been found to be good materials for organic electronics since they provide interesting features like mechanical flexibility and high impact resistance. Moreover, they offer the possibility to produce devices by low cost roll-to-roll printing techniques. Thus, they are highly promising candidates for organic thin-film transistors and solar cells. For applications, however, these materials should fulfill several demands such as ambient stability, and good film-forming properties with little change of the electronic characteristics depending on the exact molecular arrangement. The charge carrier mobility is one of the most important quantities.

In order to analyze the influence of the molecular structure on these properties, we investigate DA polymers using first-principles methods as density functional theory (DFT). In particular, density functional based tight binding (DFTB) is used to study large systems. Starting from isolated monomers being the building blocks of the DA polymers the total energy, the atomic charges, the difference between highest occupied and lowest unoccupied molecular orbitals, and the reorganization energies are obtained, and the transport properties are evaluated by means of complex band structure calculations. Finally, the morphological properties are explored by studying deliberately distorted systems with different angles along the backbone, and by molecular dynamics.



# Statistical studies on random configurations of silicon-germanium carbon alloys using density functional theory

Willi Roscher<sup>1</sup>, Florian Fuchs<sup>2,4,5</sup>, Christian Wagner<sup>2,3</sup>, Jörg Schuster<sup>2,4,5</sup>, and Sibylle Gemming<sup>2,3</sup>

<sup>1</sup> Leibniz Institute for Solid State and Materials Research Dresden, Dresden, Germany

<sup>2</sup> Institute of Physics, Technische Universität Chemnitz, Chemnitz, Germany

<sup>3</sup> Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Dresden, Germany

<sup>4</sup> Fraunhofer Institute for Electronic Nano Systems (ENAS), Chemnitz, Germany

<sup>5</sup> Center for Microtechnologies, Technische Universität Chemnitz, Chemnitz, Germany

Random alloys are relevant for many applications. One example is silicon-germanium carbon which is used for high frequency devices like heterojunction-bipolar transistors. We therefore investigate the electronic structure of  $\text{Si}_{1-x-y}\text{Ge}_x\text{C}_y$  alloys in the entire composition range  $0 \leq x \leq 1$  and small C concentrations. For our study we use density functional theory in combination with bulk models of the alloys. To describe the band gap precisely we use the pseudopotential projector shift method as implemented in QuantumATK 18.06. We perform a random generation of  $\text{Si}_{1-x-y}\text{Ge}_x\text{C}_y$  structures to get statistical distributions of the electronic properties. After optimizing the structure we evaluate the band structure by averaging equivalent directions in the Brillouin zone. The mean of the band gap is in good agreement with experimental reference data. We also demonstrate wide variations of the band gap, which are in the range of about 10 %. Further properties, such as the lattice constant, the formation energy and the change of Gibbs free energy are studied as well. For application-relevant structures a concentration gradient in  $\text{Si}_{1-x}\text{Ge}_x$  was applied and results in local changes of the band gap.

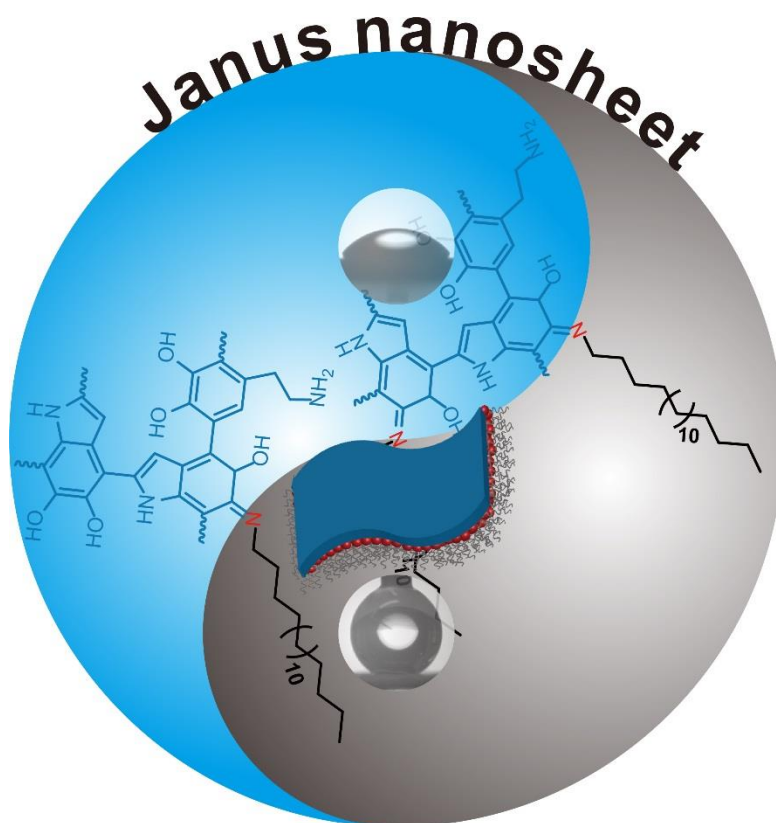
# Mussel- Inspired Two- Dimensional Freestanding Alkyl- Polydopamine Janus Nanosheets

Wenbo Sheng, Rainer Jordan\*

Chair of Macromolecular Chemistry, Faculty of Chemistry and Food Chemistry, Technische Universität Dresden, Mommsenstr. 4, 01069 Dresden, Germany

Corresponding author: Rainer.Jordan@tu-dresden.de

Mussel- inspired two- dimensional freestanding, alkyl- polydopamine (alkyl- PDA) Janus nanosheets, with a well- controlled nanometer thickness and a lateral size of up to micrometers, have been developed. A self- assembled octadecylamine (ODA) bilayer is used as the reactive template for the dopamine polymerization, resulting in the formation of well- defined nanosheets. The alkyl- PDA nanosheets show an amphiphilic nature with hydrophilic PDA and hydrophobic alkyl chains on opposing sides. The nanosheets can be used to functionalize many substrates and is dependent on the configuration of surface of the nanosheets. The nanosheets are quite stable, as the morphology is preserved after carbonization at 900 °C. Post- modification of the nanosheets can be easily achieved because of the reactive nature of PDA. This work will provide a new strategic approach for fabricating polymeric Janus nanosheets, which can find applications for surface modifications, catalyst supports, and guided self- assembly.



# Resistivity and Mobility Evolution of Monolayer Graphene at Different Degree of Arylation

Martin Siebert<sup>1</sup>, Maria Kolešnik-Gray<sup>1</sup>, Daniela Dasler<sup>2</sup>,

Katja Maurer-Chronakis<sup>2</sup>, Frank Hauke<sup>2</sup>, Andreas Hirsch<sup>2</sup>, Vojislav Krstić<sup>1</sup>

<sup>1</sup> Department of Physics, Friedrich-Alexander-Universität (FAU) Erlangen-Nürnberg,  
Staudtstraße 7, 91058 Erlangen, Germany

<sup>2</sup> Department of Chemistry and Pharmacy & Joint Institute of Advanced Materials and  
Processes (ZMP), Friedrich-Alexander-Universität (FAU) Erlangen-Nürnberg,  
Henkestrasse 42, 91054 Erlangen, Germany

Corresponding author: martin.siebert@fau.de

The modification of graphene by chemical means offers novel functionalities and properties for potential applications. In the present work, we studied the electrical properties of monolayer graphene arylated with iodonium salts. We observed a strong increase of resistivities and decrease of charge carrier mobilities with increasing degree of functionalization. We compared these with Raman measurements to gain insight into the nature of potential scattering mechanisms. From the ratios of intensities of the D, D' and G-lines we can attribute, if inter-valley or intra-valley electron-phonon scattering is the dominant process or if both are equally present.

# Phase Sensitive Transmission of Light Through Germanium Nanohelices

Janis Sperga<sup>1</sup>, Günter Ellrott<sup>2</sup>, Sergej Rothau<sup>1</sup>, Norbert Lindlein<sup>1</sup>, Vojislav Krstić<sup>1</sup>

<sup>1</sup>Department of Physics, Friedrich-Alexander Universität (FAU) Erlangen-Nürnberg,  
Staudtstrasse 7, 91058 Erlangen, Germany

<sup>2</sup> School of Material Science, Japan Advanced Institute of Science and Technology (JAIST),  
1-1 Asahidai, 923-1292 Nomi, Ishikawa, Japan

Corresponding author: vojislav.krstic@fau.de

Nanohelices represent a class of optically active chiral metamaterials which can be fabricated using GLAD (Glancing angle deposition). With this method, the size and shape of nanohelices can be controlled. Due to their specific geometry, the optical properties of nanohelices are polarization-sensitive, e.g., they exhibit a circular birefringence and circular dichroism due to their chirality.

In the present work, we produced a vertical array of germanium nanohelices grown on a transparent SiC substrate. Using polarization and phase shifting interferometry, [1] we measured the change of polarization state (that is, the ellipticity and the rotation angle of polarization vector) of light passing through the nanohelix system.

We observed both a significant linear and circular birefringence of germanium nanohelices.

## References:

- [1] S. Rothau, C. Kellermann, S. Mayer, K. Mantel, and N. Lindlein, "Polarization and phase-shifting interferometry for arbitrary, locally varying polarization states," *Applied Optics*, vol. 56, no. 5, pp. 1422-1430, 2017.

## **Microwave Studies of Graphene/hBN Heterostructures**

Vincent Strenzke<sup>1</sup>, Udai R Singh<sup>1</sup>, Chithra H Sharma<sup>1</sup>, Marta Prada<sup>2</sup>, Lars Tiemann<sup>1</sup>,  
Robert H Blick<sup>1</sup>

<sup>1</sup>Center for Hybrid Nanostructures, Universität Hamburg, Hamburg, Germany

<sup>2</sup>I. Institute for Theoretical Physics, Universität Hamburg, Hamburg, Germany

Corresponding author: [vsstrenzk@physnet.uni-hamburg.de](mailto:vsstrenzk@physnet.uni-hamburg.de)

The band structure of monolayer graphene exhibits a small band gap in the range of tenth of  $\mu\text{eV}$  that results from intrinsic spin orbit interaction. To probe such low energies in magnetotransport experiments at cryogenic temperatures, a resistively detected microwave resonance method can be employed. In this work, graphene was combined with hexagonal boron nitride (hBN), i.e., a two-dimensional material which is a superior substrate for high-quality electronics as compared to silicon substrates. In these Graphene/hBN heterostructures, we observed additional features in the microwave resonance spectrum, signalling additional interactions and phenomena. Combining graphene with other two-dimensional van der Waals materials such as  $\text{MoS}_2$  offers a variety of possibilities for further fundamental studies.

## FeSe growth on Se-rich Bi<sub>2</sub>Se<sub>3</sub> surfaces: Growth dynamics, structure, and electronic properties

M. Vondráček<sup>1</sup>, J. Fikáček<sup>1</sup>, V. Stetsovych<sup>4</sup>, P. Procházka<sup>3</sup>, S. Průša<sup>3</sup>, L. Kormoš<sup>3</sup>,  
J. Čechal<sup>3</sup>, O. Caha<sup>3</sup>, G. Springholz<sup>4</sup>, and J. Honolka<sup>1</sup>

<sup>1</sup>*Institute of Physics, Academy of Sciences of the Czech Republic, Na Slovance 2,  
182 21 Prague 8, CZ*

<sup>2</sup>*Department of Condensed Matter Physics, Faculty of Mathematics and Physics,  
Charles University, Ke Karlovu 2, 121 16 Prague 2, CZ*

<sup>3</sup>*CEITEC - Central European Institute of Technology, Brno University of Technology,  
Purkyňova 123, 612 00 Brno, CZ*

<sup>4</sup>*Institut für Halbleiter- und Festkörperphysik, Johannes Kepler Universität,  
Altenbergerstraße 69, 4040 Linz, Austria*

Corresponding author: vondrac@fzu.cz

FeSe van der Waals crystals show *unconventional* superconductivity below a critical temperature of  $T_c = 8$  K. The origin of unconventional superconductivity is still discussed controversially. In the last years the interest in Fe-chalcogenide superconductors has intensified after the critical temperature of FeSe was reported enhanced by more than one order of magnitude in the monolayer limit in the presence of non-conductive oxide substrate interfaces. For an overview see ref. [1].

So far superconductive properties were mostly studied by local scanning tunneling spectroscopy (STS) experiments. Macroscopic transport properties were rarely reported since respective experiments require continuous films with homogeneous material properties. Here we report on recent progress in growth of 2D FeSe layers on Bi<sub>2</sub>Se<sub>3</sub> topological insulator (TI) surfaces and subsequent overlayer growth using e.g. oxides and Si adlayers. In order to reduce shunt currents in transport we keep TI substrate thicknesses in the tens of nanometer range, which is achieved by molecular beam epitaxy (MBE). Growth dynamics, structure, and electronic properties of FeSe prepared under Se-rich conditions are analyzed in depth by scanning tunneling microscopy (STM), angle resolved photoemission spectroscopy (ARPES), low-energy electron microscopy (LEEM), and low-energy ion scattering spectroscopy (LEIS). In contrast to growth reports on flat bulk TI crystals [2,3] (terrace width ~100 nm), we observe a strong influence of the high step-edge density (terrace width ~10 nm) in MBE-grown TI surfaces, which significantly promotes FeSe growth.

[1] X. Liu et al., *J. Phys.: Condens. Matter* **27**, 183201 (2015)

[2] F. Arnold et al., *J. Phys.: Condens. Matter* **30**, 065502 (2018)

[3] A. Eich et al., *Phys. Rev. B* **94**, 125437 (2016)

## **Towards an enhancement of the magnetoresistance in monolayer graphene with metallic superlattices**

Agastya Wiraputra<sup>1</sup>, Benjamin Hacker<sup>1</sup>, Vojislav Krstić<sup>1</sup>

<sup>1</sup>Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Erlangen, Germany

Corresponding author: [vojislav.krstic@fau.de](mailto:vojislav.krstic@fau.de)

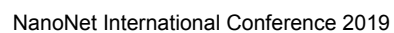
Graphene can be modified in order to control and tune its electrical properties under magnetic field influence. One way to modify its characteristics is by introducing impurities on top of this two dimensional material. With this introduction of impurities, the physical properties are accordingly altered and this work aims to alter the properties of graphene under as it normally shows low magnetoresistance behavior. In this work, a periodic array of metal discs is deposited on an exfoliated monolayer graphene as a way to modify its properties. It is shown in our measurements that this approach is indeed a feasible way to steer and potentially enhance the magnetoresistance in monolayer graphene.

## Your Notes



## Your Notes

blue dot: Pier for Boat tour and Dinner (Thursday 5:30 pm.)



## NanoNet International Conference 2019, Dresden

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Updated: 02.10.2019 (PZ)

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Arora	Himani	Ms.		HZDR
Au Yeung	Kwan Ho	Mr.		TU Dresden
Banerjee	Semanti	Ms.		IPF Dresden
Bayrak	Turkan	Ms.		HZDR
Belyayev	Dmitry	Mr.		TU Dresden
Bol	Ageeth	Ms.	Prof. Dr.	Eindhoven TU
Braun	Hans-Georg	Mr.	PD Dr.	IPF Dresden
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Ditte	Kristina	Ms.		IPF Dresden
Echresh	Ahmad	Mr.		HZDR
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Kolešnik-Gray	Maria	Ms.	Dr.	FAU Erlangen/Nürnberg
Krstić	Vojislav	Mr.	Prof. Dr.	FAU Erlangen/Nürnberg
Kühne	Tim	Mr.	MSc.	TU Dresden
Lissel	Franziska	Ms.	Dr.	IPF Dresden
Lokamani	Mani	Mr.	Dipl.-Ing.	HZDR
Lopushanska	Bohdana	Ms.		U Uzhgorod
Metzger	Robert	Mr.	Prof. Dr.	U Alabama
Meyer	Jana Marie	Ms.	BSc.	U Hamburg
Moresco	Francesca	Mrs.	Dr.	TU Dresden
Ortmann	Frank	Mr.	Dr.	TU Dresden
Perumallapelli	Goutham Raj	Mr.		IPF Dresden
Porath	Danny	Mr.	Prof. Dr.	U Jerusalem
Preis	Kevin	Mr.		TU Chemnitz
Pump	Florian	Mr.		TU Dresden
Roscher	Willi	Mr.		IPF Dresden
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Seifert	Gotthard	Mr.	Prof. Dr.	TU Dresden
Sheng	Wenbo	Ms.		TU Dresden
Siebert	Martin	Mr.		FAU Erlangen/Nürnberg
Singh	Parminder	Mr.		HZDR
Solovev	Anton	Mr.		TU Dresden
Sperga	Janis	Mr.		FAU Erlangen/Nürnberg
Strenzke	Vincent	Mr.	BSc.	U Hamburg
Strobel	Alexander	Mr.		HZDR
Vondráček	Martin	Mr.	Mgr.	CAS Prague
Wiraputra	Agastya	Mr.		FAU Erlangen/Nürnberg
Zahn	Manuel	Mr.		HZDR
Zahn	Peter	Mr.	PD Dr.	HZDR
Zessin	Johanna	Ms.		U Jerusalem
Zhuravel	Roman	Mr.		U Jerusalem

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