International Helmholtz Research School for Nanoelectronic Networks



## **IHRS NANONET International Workshop 2016**

## 30 August – 02 September 2016

## Prague, Czech Republic



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nancelectronic materials laboratory



## Venue and organization

## Venue

Hotel Angelo Prague (by Vienna House) Radlická 1g 15000 Prague 5, Czech Republic Phone: +420 234 801 111 E-mail: info.angelo-prague@viennahouse.com Homepage: www.viennahouse.com/en/angelo-prague/

## Organization

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

## **Local Organizers**

PD Dr. Peter Zahn Institute of Ion Beam Physics and Materials Research Helmholtz-Zentrum Dresden-Rossendorf 01328 Dresden, Germany Phone: +49 351 260 3121 E-mail: nanonet@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

Dr. Jan Honolka Institute of Physics Czech Academy of Sciences (CAS) Na Slovance 2, 182 21 Prague 8 Czech Republic Phone: +420 26605 2389 E-mail: honolka@fzu.cz

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#### NanoNet International Workshop 2016, Prague

#### Agenda

Place: Hotel Angelo, Radlicka 1g, 15000 Prague 5 updated: 26.08.2016 (PZ)



#### Tuesday, 30 August 2016

Start	Who	Durat.	Short Title (Full titles see next page)	Notes
8:40			Bus transfer from Dresden-Hauptbahnhof	
12:00			Arrival/Lunch Buffet	Chair: P. Zahn
13:30	A. Erbe		Welcome address	
13:40	D. Porath	40+10	Charge Transport in DNA-Based Molecules (Introductory Le	ecture)
14:30	H. Vazquez	40+10	Calculation of elastic & inelastic electron transport in single	molecule junctions
15:30		30	Break	Chair: H. Vazquez
16:00	E. Lörtscher	40+10	Singe-Molecule Electronics and Optics	
17:00		120	Poster session	27 Posters
19:30			Dinner	
Wednesday, 31 August 2016				Chair: V. Krstic
8:45	H. Mizuta	40+10	Graphene-based nanoelectronic and nano-electro-mechan	ical devices
9:35	E. Baek	20+10	Negative photoconductivity of highly doped Si nanowire FE	
10:30		30	Break	Chair: M. Lörtscher
11:00	D. Porath	40+10	Charge Transport in single Adsorbed Long DNA-Based Mo	
11:50	A. Stern	20+10	Electrical Characterization of 1D Molecular Structures	
12:30			Lunch	Chair: D. Porath
14:00	N. Fardian-Melamed	20+10	STM and Spectroscopy of Novel Silver-Containing DNA Mo	lecules
14:30	J. Honolka	20+10	SAFMAT: Materials science and facilities	
15:00	I. Kratochvilova	20+10	FUNBIO: scope, instruments, results	
15:30	1. 144061111074	30	Break	
16:00		00	Sightseeing (starting at the hotel lobby)	
19:30			Free Time	
Thursday, 01 September 2016				Chain C. Caifart
Thurse	uay, uh September 201	0		Chair: G. Seifert
			Mechanical properties of fluctuating graphene membranes	Chair: G. Sellen
8:45	J. Gomez V. Krstic	40+10	Mechanical properties of fluctuating graphene membranes Transport in nanowires and nanowire-based devices	Chair: G. Seiren
	J. Gomez		Transport in nanowires and nanowire-based devices	Chair: V. Bouchiat
8:45 9:35	J. Gomez	40+10 40+10		Chair: V. Bouchiat
8:45 9:35 10:30	J. Gomez V. Krstic	40+10 40+10 30	Transport in nanowires and nanowire-based devices Break	Chair: V. Bouchiat
8:45 9:35 10:30 11:00	J. Gomez V. Krstic M. Kolesnik-Gray	40+10 40+10 30 20+10	Transport in nanowires and nanowire-based devices Break Size-dependent charge transport in Au-seeded Ge nanowir	Chair: V. Bouchiat
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Breakfast will be served from 6:30.

## **Invited Talks**

**Bogani, Lapo** (p. 4) Graphene-based nanomaterials for molecular spintronics

**Bouchiat, Vincent** (p. 5) Collective behavior of physisorbed active elements on Graphene: from 2D superconducting transitions to neural network bio-applications

**Gomez-Herrero, Julio** (p. 6) Mechanical properties of fluctuating graphene membranes

**Jariwala, Deep** (p. 7) Mixed Dimensional van der Waals Heterostructures for Nanoelectronics and Photovoltaics

**Karthäuser, Silvia** (p. 8) UHV-STM investigations on three-dimensional molecules

## Krstić, Vojislav (p. 9)

Transport in nanowires and nanowire-based devices: interface, surface and confinement

**Lörtscher, Emanuel** (p. 10) Singe-Molecule Electronics and Optics

## Mizuta, Hiroshi (p. 11)

Graphene-based nanoelectronic and nano-electro-mechanical (NEM) devices for challenging applications

## Porath, Danny (p. 12)

The Quest for Charge Transport in DNA-Based Molecules (Introductory Lecture)

**Porath, Danny** (p. 13) The Quest for Charge Transport in single Adsorbed Long DNA-Based Molecules

**Seidel, Ralf** (p. 14) Self-assembly of metallic nanostructures using DNA mold templates

## Seifert, Gotthard (p. 15)

Anisotropic Thermoelectric Response in Two-dimensional Puckered Structures

## Vazquez, Hector (p. 16)

Calculation of elastic and inelastic electron transport in single molecule junctions

## **Contributed Talks**

**Baek, Eunhye** (p. 17) Negative photoconductivity of highly doped Si nanowire FETs

**Fardian-Melamed, Natalie** (p. 18) Scanning Tunneling Microscopy and Spectroscopy of Novel Silver-Containing DNA Molecules

**Honolka, Jan** (p. 19) Centre for Analysis of Functional Materials (SAFMAT): Materials science and facilities

**Kalbac, Martin** (p. 20) Chemistry on graphene

**Kolesnik-Gray, Maria** (p. 21) Size-dependent charge transport in Au-seeded Ge nanowires

**Kratochvilova, Irena** (p. 22) Centre of functional materials for bio-applications (FUNBIO): scope, instruments, results

**Stern, Avigail** (p. 23) Electrical Characterization of 1D Molecular Structures

**Teschome, Bezu** (p. 24) DNA origami nanostructures for application in nanoelectronics

**Tkáč, Vladimír** (p. 25) Magnetotransport properties of Mn-doped Bi<sub>2</sub>Se<sub>3</sub> topological insulator

**Vejpravova, Jana** (p. 26) Tailoring wrinkles in graphene by nanoparticles and fullerenes

**Zhuravel, Roman** (p. 27) Towards electrical transport measurements through single DNA molecules

## **Poster Contributions**

see list on page 28

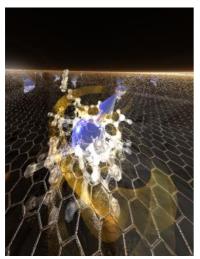
#### Graphene-nanodevices for molecular spintronics

#### L. Bogani

#### Department of Materials, University of Oxford, 16 Parks Rd. OX1 3PH, Oxford, UK

The problem of how flowing electrons interact with single spins is a fundamental one, which conceptually determines the working principles and performances of spintronic devices. The use of molecular magnets can help shed light on fundamental processes and indicate new avenues, because of the clarity with which perturbative effects can be detected. Several proposals for spintronics rely on graphene, because of its high mobility, and the possibility of injecting coherent spin currents even at room temperature. However, the influence of the graphene environment on the spin systems has yet to be unraveled, as well as how molecular systems can be used to control spin currents or single magnetic molecules.

Here we concentrate on our approach of using graphene as a conductor that can interact with molecular magnets. We first explore the spin-graphene interaction by studying the classical and quantum dynamics of molecular magnets on graphene. While the static spin



response remains unaltered, the quantum spin dynamics and associated selection rules are profoundly modulated.<sup>1</sup> We quantify the effect of the perturbed phonon environment on the classical dynamics of molecular spins, and we then show that the presence of the conduction channel can strongly alter the quantum properties. We then show how to inject coherent spin currents in graphene planes<sup>2</sup> and how molecular spins can be used to control them.<sup>3</sup> We show that the Hanle precession can be strongly influenced by the interaction with molecular spins, which can introduce an additional level of control for the spintronic response.<sup>3</sup> Eventually, we show how nanoscale gaps can be created in graphene to accommodate single molecule magnets, and what parameters dominate the anisotropy of such single-molecule spintronic devices.<sup>4</sup>

These findings provide fundamental insight into the interaction between spins and graphene, establishing the basis for electrical spin-manipulation in graphene nanodevices. A discussion for future perspective is then provided, in the light of such results.

#### References

- [1] C. Cervetti et al., Nature Mat., 2016, 15, 164-169.
- [2] C. Cervetti et al., *submitted*.
- [3] C. Cervetti et al., *submitted*.
- [4] J. Liu et al., *in preparation*.

### Collective behavior of physisorbed active elements on Graphene: From 2D superconducting transitions to neural network bio-applications

Vincent Bouchiat, Z. Han, F. Veliev, A. Allain, A. Bourrier, H. Arjmandi-Tash, A. Briançon, C. Delacour

Nanoscience Department NEEL Institute, CNRS, Université Grenoble-Alpes, Grenoble, France

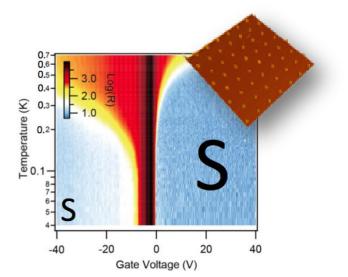
Corresponding author: bouchiat@grenoble.cnrs.fr

Graphene provides an ideal 2D gas of Dirac Fermions, which is directly exposed to the environment. Therefore it provides an ideal platform on which to tune, via application of an electrostatic gate, the electronic coupling between ordered adsorbates deposited on its surface via the control of density and sign of charge carriers. This situation is particularly interesting when the network of adsorbates are actively interacting between each other and can induce some long range electronic order within the underlying graphene substrate, such as superconducting correlations [1]. To demonstrate this concept, we have measured arrays of superconducting clusters physisorbed on Graphene capable to induce via the proximity effect a gate-tunable superconducting transition. We have experimentally studied the case of macroscopic graphene decorated with an array of superconducting tin clusters [2], which induce via percolation of proximity effect a global but tunable 2D superconducting state. By adjusting the graphene disorder and its charge carrier density on one side, the geometrical order, cluster size and density of the superconducting dot network on the other side, the superconducting state can exhibit very different behaviors, allowing to test different regimes and quantum phase transition from a granular superconductor to either metallic or insulating states, leading to a bosonic-type gate-controlled quantum phase transition [3]. I will show recent experimental results involving three sets of triangular arrays sparsely distributed on graphene, in which superconductivity is destroyed for a critical gate value that we attribute to the effect of quantum fluctuations of the phase giving rise to an intermediate metallic state [4]. Finally, I will give another example of organized elements on graphene involving the interaction of in-situ grown neurons on graphene transistors.

#### References

- [1] M. Feigel'man et al., JETP Lett. **88**, 747 (2008).
- [2] B.M. Kessler et al., Phys. Rev. Lett. 104, 047001 (2010).
- [3] A. Allain et al., Nat. Mat. 11, 590 (2012).
- [4] Z. Han et al., Nat. Phys. 10, 380 (2014).
- [5] F. Veliev et al., subm. to Nano Lett. (2016).

Figure: Low temperature phase diagram of superconducting transition triangular array of Tin dots decorating graphene, inset: AFM micrograph of the corresponding sample (scan size 10 microns).



## Mechanical properties of fluctuating graphene

<u>J. Gomez-Herrero</u><sup>1</sup>, G. Lopez-Polin<sup>1</sup>, C. Gomez-Navarro<sup>1</sup>, R. Roldan<sup>2</sup>, M. Katsnelson<sup>3</sup>, F. Guinea<sup>2</sup>, Maria Ortega<sup>1</sup>, J. G. Vilhena<sup>1</sup>, and Rubén Perez<sup>1</sup>

<sup>1</sup> Dpto. Fisica Materia Condensada, Universidad Autonoma de Madrid and IFMAC, Spain <sup>2</sup> Instituto Ciencia de Materiales de Madrid, CSIC and IMDEA Nanociencia, Madrid, Spain

<sup>3</sup> Institute for Molecules and Materials, Radboud University Nijmegen, Netherlands

#### E-mail: julio.gomez@uam.es

Bendable membranes (with bending rigidity comparable to their thermal energy) exhibit entropic effects in the form of out of plane fluctuations that bring out exotic mechanical properties such as size dependent elastic constant and negative thermal expansion coefficient [1]. Graphene is the nature's thinnest elastic membrane. It is highly bendable, stiff and anharmonic. Therefore the above mentioned phenomena should apply to it.

In this work we measure, by means of indentation experiments, the dependence of the elastic modulus of graphene both as a function of controlled induced defects [2] and a as a function of external strain [3]. Our results support renormalization of the elastic constants of graphene at room temperature.

We experimentally observe that graphene stiffens up to the double of its initial value when low densities of carbon vacancies are induced. It also presents a substantial increase in Young's modulus at high external strains. We attribute these observations to the suppression of out of plane oscillations both by defects and strain.

Finally, we report experimental and theoretical evidence that point out that the negative expansion coefficient of graphene decreases in absolute value as a function of the irradiation dose supporting again the suppression of out plane oscillations with punctual defects.

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## Mixed Dimensional van der Waals Heterostructures for Nanoelectronics and Photovoltaics

#### Deep Jariwala, Dept. Applied Physics and Materials Science, CalTech, USA

The isolation of a growing number of two-dimensional (2D) materials has inspired worldwide efforts to integrate distinct 2D materials into van der Waals (vdW) heterostructures. While a tremendous amount of research activity has occurred in assembling disparate 2D materials into "all-2D" van der Waals heterostructures,<sup>1, 2</sup> this concept is not limited to 2D materials alone. Given that any passivated, dangling bond-free surface will interact with another via vdW forces, the vdW heterostructure concept can be extended to include the integration of 2D materials with non-2D materials that adhere primarily through noncovalent interactions.<sup>3</sup> In the first part of this talk I will present our work on emerging mixed-dimensional (2D + nD, where n is 0, 1 or 3) heterostructure devices performed at Northwestern University. I will present 3 distinct examples of gate-tunable p-n heterojunctions.<sup>4-6</sup> I will show that when a single layer n-type MoS<sub>2</sub> (2D) is combined with p-type semiconducting single walled carbon nanotubes (1D), the resulting p-n junction is gate-tunable and shows a tunable diode behavior with rectification ratios varied from 1-10<sup>5</sup> as a function of gate voltage and a unique anti-ambipolar transfer behavior.<sup>4</sup> Further the same concept when extended to p-type pentacene (0D) and n-type 2D MoS<sub>2</sub> leads to a tunable p-n junction with a photovoltaic effect and an asymmetric anti-ambipolar transfer response.<sup>6</sup> I will present the underlying charge transport and photocurrent responses in both the above systems using a variety of scanning probe microscopy techniques as well as computational analysis. Finally, I will show that the anti-ambipolar field effect observed in the above two systems can be generalized to other semiconducting heterojunction systems and extended over large areas with practical applications in simplification of wireless communication circuits.<sup>5</sup>

The second part of talk will discuss my more recent work performed at CalTech on photovoltaic devices from 2D semiconductors such as transition metal dichalcogenides (TMDCs). High efficiency inorganic photovoltaic materials (e.g., Si, GaAs and GaInP) can achieve maximum above-bandgap absorption as well as carrier-selective charge collection at the cell operating point. But thin film photovoltaic absorbers have lacked the ability to maximize absorption and efficient carrier collection, often due to due to surface and interface recombination effects. In contrast, Van der Waals semiconductors have naturally passivated surfaces with electronically active edges that allows retention of high electronic quality down-to the atomically thin limit. I will show experimental demonstration of near-unity light absorption in extremely thin (< 15 nm) Van der Waals semiconductor ( $MoS_2$ ,  $WS_2$  and  $WSe_2$ ) structures by coupling to strongly damped optical modes of semiconductor/metal heterostructures. I will further present the fabrication and performance of our, broadband absorbing photovoltaic devices using sub-15 nm thick transition metal dichalcogenides (TMDCs) as the active layers. Our TMDC devices show a short circuit current density > 10 mA/cm<sup>2</sup> at ~20 Suns and exhibits spectral response that parallels the spectral absorption over the above bandgap region.<sup>7</sup> I will conclude by presenting future prospects for TMDCs and other 2D materials as well as their heterostructures in photovoltaics and electronic applications. References:

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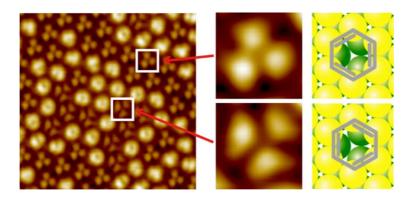
### **UHV-STM** investigations on three-dimensional molecules

<u>Silvia Karthäuser</u><sup>1</sup>, Michael Paßens<sup>1</sup>, Rene Ebeling<sup>1</sup>, Nicolae Atodiresei<sup>2</sup> <sup>1</sup>Peter Grünberg Institut (PGI-7) and JARA-FIT, Forschungszentrum Jülich GmbH, D-52425 Jülich, Germany <sup>2</sup>Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich GmbH, D-52425 Jülich, Germany

Corresponding author: s.karthaeuser@fz-juelich.de

Fullerenes on metallic substrates are very rich systems with respect to their rotational degrees of freedom and possible interactions with different adsorption sites or next neighbors. Using these three-dimensional molecules as a first example, the advantages of voltage dependent imaging to identify molecular orbitals will be shown. Another focus will be the ability of fullerenes to form self-assembled monolayers that mirror impressively the electronic properties of the respective substrate. Even second order interface effects, that is, the interactions of fullerenes with atoms of the subsurface layer are identified (Fig. 1).

As a second three-dimensional molecule N,N'-dibenzyl-naphthoic bisimide, which consists of a large  $\pi$ -conjugated backbone and two phenyl-rings each connected with a methylene-linker to the central part, will be presented here. Both, the conformation of a single molecule adsorbed on a Pt(111) substrate and the orbital symmetry can be deduced. Most interestingly, according to the high resolution UHV-STM images, the naphthoic bisimide backbone of the molecule adsorbs flat on the substrate and nitrogen atoms show up as bright spots. Moreover, the two benzyl groups build one line together with the backbone and electron densities on both sides of the phenyl rings can be identified. In addition, the orbital symmetry of the HOMO and the LUMO identified by UHV-STM was compared to DFT based calculations on N,N'-dibenzyl-naphthoic bisimide part with a phenyl group results in a protruding phenyl group while the larger conjugated system adsorbs on the substrate.



# Transport in nanowires and nanowire-based devices: interface, surface and confinement

#### Vojislav Krstić

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

Corresponding author: vojislav.krstic@fau.de

As quasi-1D nanostructures, nanowires represent an intriguing electronic system in which the full range from semi-classical to quantum-determined transport can be observed. Which of the aforementioned transport regimes and associated phenomena establishes, depends in particular on scattering at interfaces and doping from surfaces, the confinement of the charge-carriers within the wires, the material the nanowire is made of (metal or semiconductor), and how it was synthesised (e.g. self-seeded or catalytic-seed driven). Moreover, due to the nanosized dimensions of the nanowire, all these aspects can mutually depend on each other. Regarding devices, even the (local) device geometry into which a nanowire is integrated to has impact on the overall nanowire-device performance (e.g., contact resistivity, sensor proper ties). This is of crucial importance for any application of nanowires and further development of nanowire-based technology platforms.

In the present work, experimental studies on individual synthetic Ag and Ge nanowires will be presented. The chosen examples will demonstrate the rich variety in transport phenomena encountered in nanowire(-devices) depending on the surfaces, interfaces, doping and confinement, spanning the range from intrinsic (material-specific) to extrinsic (device-layout) driven properties.

### **Single-molecule Electronics and Optics**

Emanuel Lörtscher

IBM Research – Zurich, Säumerstrasse 4, CH-8803 Rüschlikon

#### eml@zurich.ibm.com

The vision of molecular electronics is to employ single molecules as functional building blocks in electronic circuits.<sup>[1]</sup> Various candidates are characterized using a mechanically controllable breakjunction and a statistical measurement procedure.<sup>[4]</sup> Besides current rectification<sup>[2]</sup> conductance switching is one fundamental operation required for electronic applications. Organometallic compounds<sup>[3]</sup> with embodied redox-active metal centers are a promising novel class of functional molecules as they do not need to undergo conformational changes upon changing their redox state. Compounds bearing Fe, Ru or Mo metal centers with an extensive charge-delocalization over the entire unsaturated organometallic backbone<sup>[5]</sup> are equipped with various anchoring schemes<sup>[6]</sup> including direct  $\sigma$ -bonds.<sup>[7]</sup> A strong hybridization of metal states and molecular orbitals as in case of direct C-Au bonds leads to a high conductance but prohibits intrinsic redox degrees of freedom.<sup>[8]</sup> By reducing the coupling strength in S-(4ethynylphenyl)-ethanethioate anchored bis( $\sigma$ -arylacetylide) complexes, voltage-induced conductance switching can be preserved. In case of Mo, the pronounced and abrupt switching with on/off conductance ratios up to 400<sup>[9]</sup> will be discussed by DFT and a two-channel transport mechanism that can also be found in purely organic Azulene derivatives.[10]

In the second part, bottom-up and directed integration of ensemble of molecules on a planar Silicon platform will be shown. By selective etching of a stack of various oxides, vertical nanopores can be fabricated on atomically-flat bottom electrodes<sup>[11]</sup> to act as compartments for the self-assembly of molecules for applications in molecular electronics but also in molecular factories.<sup>[12]</sup> Transport properties of alkane-dithiols will be reported revealing 3 orders of magnitude reduced conductance fluctuations in these fixed-gap devices, accompanied with the expected exponential decay in conductance as a function of molecular length. In contrast to break-junction measurements that require UHV and cryogenic temperatures, this ensemble platform can be operated under ambient conditions which represents a significant step towards the integration of molecular building blocks on a technologically relevant platform.

In the last part, fabrication of ultra-narrow gaps<sup>[13]</sup> with sub-5nm in-plane separation achieved by electronbeam lithography under ultra-silent conditions<sup>[14]</sup> will be demonstrated. This approach does no more require mechanical actuation to establish small gaps between the electrodes and can furthermore be used to create plasmonic antennas for single-molecule spectroscopy based on Raman scattering.

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## Graphene-based nanoelectronic and nano-electromechanical (NEM) devices for challenging applications

<u>Hiroshi Mizuta<sup>1,2,3</sup></u>, Ahmed Hammam<sup>1</sup>, Jothiramalingam Kulothungan<sup>1</sup>, Shunei Suzuki<sup>1</sup>, Marek E. Schmidt<sup>1</sup>, Jian Sun<sup>1</sup> and Manoharan Muruganathan<sup>1</sup>

<sup>1</sup> Energy and Environmental Research Division, School of Materials Science, Japan Advanced Institute of Science and Technology (JAIST), Nomi, Japan

<sup>2</sup> Nanoelectronics and Nanotechnologies Group, ECS, Faculty of Physical Sciences and Engineering, Univ. of Southampton, Southampton, UK

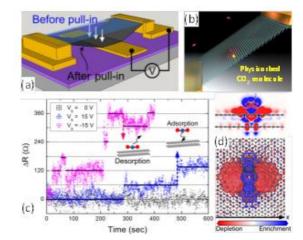
<sup>3</sup> Institute of Microengineering and Nanoelectronics (IMEN), The National University of Malaysia, Selangor, Malaysia

Corresponding author: mizuta@jaist.ac.jp

Graphene possesses remarkable electronic and mechanical properties and provides a promising platform to explore future nanoelectronic and nano electro-mechanical (NEM) devices for challenging applications. A brief overview is presented for our recent attempts of developing novel graphene-based nanoscale devices. We first present state-of-the-art fabrication technology for sub-10-nm graphene nanostructures using atomic-size focused helium ion beam. Secondly graphene-based tunnel FETs (GTFETs) and graphene single carrier transistors (GSCTs) are discussed, which are expected to achieve advanced switching characteristics in comparison with conventional MOSFETs. Recent progress is shown for fabrication and characterization of the GTFETs with a very narrow graphene nanoribbon (GNR) of 15 nm in width and multiple top gates to form an electrostatically controlled PN junction. We then describe novel graphene NEM (GNEM) devices for low-voltage switching and ultra-sensitive chemical gas sensing applications. Doubly-clamped and cantilever GNEM switches with a local top actuation electrode are developed, which achieve a pull-in voltage less than 5 V. A naturally formed chromium oxide, introduced at the graphene-electrode contact interface, prevents the formation of C-Au chemical bonds, and the reversible switching operation is achieved. A GNEM chemical gas sensor device is demonstrated, which features a

slanted BLG channel with built-in tensile strain (Fig. 1). By applying a substrate bias voltage to accelerate the  $CO_2$  gas molecule adsorption processes, we show 'quantized' increments in the temporal resistance, which signifies single  $CO_2$  molecule adsorption / desorption events onto the BLG channel surface.

This work was supported by the Grant-in-Aid for Scientific Research No. 25220904 from Japan Society for the Promotion of Science (JSPS) and the Center of Innovation Program from Japan Science and Technology Agency (JST).



**Fig. 1**. (a) A schematic GNEM sensor before and after pullin. (b) An artist's impression of a  $CO_2$  gas molecule physisorbed onto the BLG. (c) Observed temporal resistance change of the GNEM sensor. (d) Cross-sectional and top-viewed charge-density difference distribution.

## The Quest for Charge Transport in DNA-Based Molecules Danny Porath

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

Email: danny.porath@mail.huji.ac.il

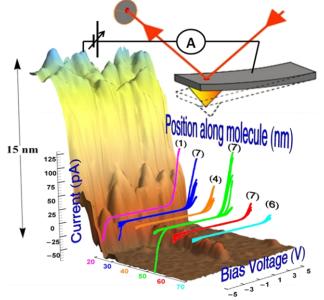
DNA and DNA-based polymers have been at the focus of molecular electronics owing to their programmable structural versatility. The variability in the measured molecules and experimental setups has produced a wide range of partial or seemingly contradictory results, highlighting the challenge to transport significant current through individual DNA-based molecules. I will review examples of the various results obtained by different groups, highlighting the effect of different conditions on the charge transport results, the different approaches to measuring charge transport, some of the modifications of DNA-based molecules and some central and important issues for understanding the obtained results.

## The Quest for Charge Transport in single Adsorbed Long DNA-Based Molecules

#### **Danny Porath**

Institute of Chemistry and Center for Nanoscience and Nanotechnology, The Hebrew University of Jerusalem, 91904 Israel danny.porath@mail.huji.ac.il

DNA and DNA-based polymers have been at the focus of molecular electronics owing to their programmable structural versatility. The variability in the measured molecules and experimental setups has produced a wide range of partial or seemingly contradictory results, highlighting the challenge to transport significant current through individual DNA-based molecules. I will report on detailed and reproducible charge transport measurements in G4-DNA, adsorbed on a mica substrate. Using a special setup for testing molecular conductance in single polymers, we observed currents of tens to over 100 pA in many G4-DNA molecules over distances ranging from tens to over 100 nm, compatible with a long-range thermal hopping



between multi-tetrad segments. With this report, we answer a long-standing question about the ability of individual polymers to transport significant current over long distances when adsorbed a hard substrate, and its mechanism. Furthermore, I will report on a new type of selectively metalized DNA. This new type of wire together with the above results may re-ignite the interest in DNA-based wires and devices towards implementing these wires in devices and programmable circuits.

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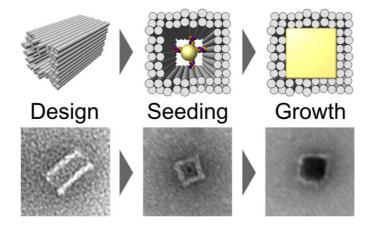
## Self-assembly of metallic nanostructures using DNA mold templates

Ralf Seidel<sup>1</sup>, Seham Helmi<sup>1</sup>, Jingjing Ye<sup>1</sup>

<sup>1</sup>Molecular Biophysics group, Institute for Experimental Physics I, Universität Leipzig, Germany

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

Biomolecule-templated synthesis of metallic and semiconducting nanostructures is a fascinating concept, where a biomolecule shall dictate the shape of the resulting inorganic nanostructure. Established procedures face, however, still important limitations, which are the rather small variety of available structures (when considering protein templates) and difficulties in achieving a fine and homogenous material deposition (in particular for DNA). Meanwhile DNA nanotechnology offers to design and fabricate a broad range of structures with complex geometries that are of high interest for biomolecular templating. To achieve a reliable and shapecontrolled synthesis of metallic nanoparticles, we developed an approach, in which such DNA structures are used as molds that become filled with a material of interest. The mold cavity thus imprints its shape onto the growing particle and also limits its growth. Furthermore, the individual molds can be used as bricks that can be stacked together to form mold superstructures. As a proof of principle we demonstrate the mold-templated synthesis of um-long gold nanowires comprising dozens of individual molds. Furthermore, we designed a number of additional mold elements that e.g. can act as caps and junctions. Using such differently shaped molds, the brickapproach will allow us in future to obtain a broad range of different geometries based on only a few building blocks. Suitable modifications within the individual molds will also allow the integration semiconducting nanostructures within a single structure and thus open the way to fabrication of simple nanoelectronic devices by just using self-assembly.



#### Anisotropic Thermoelectric Response in Two-dimensional Puckered Structures

<u>Gotthard Seifert</u><sup>1</sup>, Leonardo Medrano Sandonas<sup>2,3</sup> David Teich<sup>1</sup>, Rafael Gutierrez<sup>2</sup> Tommy Lorenz<sup>1</sup>, Alessandro Pecchia<sup>4</sup>, and Gianaurelio Cuniberti<sup>2</sup> <sup>1</sup>Theoretische Chemie, TU Dresden, 01062 Dresden, Germany

<sup>2</sup>Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden,

01062 Dresden, Germany

<sup>3</sup>Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany

<sup>4</sup>Consiglio Nazionale delle Ricerche, ISMN, Via Salaria,00017 Monterotondo, Rome, Italy

#### Abstract

Two-dimensional semiconductor materials with puckered structure offer a novel playground to implement nanoscale thermoelectric, electronic, and optoelectronic devices with improved functionality. Using a combination of approaches to compute the electronic and phonon band structures with Green's function based transport techniques, we address the thermoelectric performance of phosphorene, arsenene, and SnS monolayers. In particular, we study the influence of anisotropy in the electronic and phononic transport properties and its impact on the thermoelectric figure of merit ZT. Our results show no strong electronic anisotropy, but a strong thermal one, the effect being most pronounced in the case of SnS monolayers. This material also displays the largest figure of merit at room temperature for both transport directions, zigzag (ZT ~ 0.95) and armchair (ZT ~ 1.6), thus hinting at the high potential of these new materials in thermoelectric applications.

# Calculation of elastic and inelastic electron transport in single molecule junctions

<u>H. Vázquez</u>

Inst. of Physics, Academy of Sciences of the Czech Republic, Prague, CZ

#### vazquez@fzu.cz

Single molecule junctions are exciting nanoscale systems where a series of quantum phenomena can be explored [1]. In this talk I will give an overview of the recent work on the elastic and inelastic conductance of molecular circuits carried out in our group. We study these properties using Density-Functional Theory and Non-Equilibrium Green's Functions.

In the first part of my talk I will discuss the important role of metal-molecule links on electron transport [2]. I will compare Au-S, Au-SMe and Au-NH2 anchoring groups to direct Au-C links. These covalent Au-C bonds are formed in-situ between the tip and the terminal molecular C atoms and were shown to be highly-conducting [3]. I will discuss the signature in conductance of these metal-molecule links and examine their behavior under an applied bias.

I will then describe our work on inelastic electron tunneling spectroscopy. Here, the main physical mechanism is the interaction between the tunneling electrons and the vibrational degrees of freedom. For a representative conjugated molecule with a low degree of symmetry, we study the spatial origin of the inelastic signal and calculate, for all modes, the different contributions that give rise to the vibrational spectrum. These intra- and inter-atomic contributions involve products of scattering states with electron-phonon matrix elements and thus encode both electronic as well as vibrational information. By mapping the pattern of addition or cancellation of these partial contributions, we can draw across all vibrational modes a quantitative relation between the degree of symmetry of each mode, the strength of its inelastic signal and the locality of selection rules [4].

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## Negative photoconductivity of highly-doped Si nanowire field-effect transistors

Eunhye Baek,<sup>1</sup> Taiuk Rim,<sup>2</sup> Larysa Baraban,<sup>1</sup> Gianaurelio Cuniberti<sup>1,3</sup>

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

2 Department of Creative IT Engineering, Pohang University of Science and Technology, 37673 Pohang, Republic of Korea

3 Center for Advancing Electronics Dresden, TU Dresden, 01062 Dresden, Germany eunhye.baek@nano.tu-dresden.de

#### Abstract

The negative photoconductivity is very rare effect because of the photoexcitation of charge carriers in materials which normally enhances channel conductivity. Recently, 0- or 1-dimensional nanostructured materials have shown reduced photoconductivity due to the surface effect such as surface plasmonic change in Au nanoparticles [1], photon assisted oxygen desorption on the surface in p-type ZnSe nanowires [2] and light induced hot-electron trapping of oxide surface in n-type InAs nanowires [3]. However, the negative photoconductivity of doped Si nanowire devices has not been reported yet in spite of the enormous research and industrial demands of Si nanowires for photovoltaic and solar cell application.

In this study, we have studied the negative photoconductivity (NPC) of Si nanowire FETs (Fig. 1(a)) with different doping concentration. N-doped devices show NPC behavior unlike undoped devices which have normal positive photoconductivity (PPC) by photoexcitation of electrons in Si NWs (Fig. 1(b)). The NPC originates from the number of channel carriers trapped by dopants which are tuned by gate bias. The distinguishing feature of NPC of doped Si NWs is that the impurity trap is dominant source apart from the interfacial trap, contrary to other nanostructures. In addition, we have investigated NPC change with various illumination intensity and wavelength of light. Finally, the NPC and the PPC components are extracted respectively, which have exponential dependency with light power intensity. This study would be very promising for both tunable optoelectronics and sensor application by surface charge engineering with functional molecules.

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#### Figures

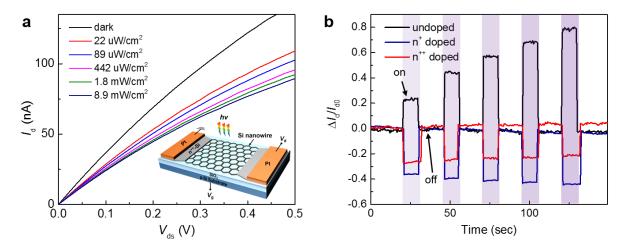


Figure 1 (a)  $I-V_{ds}$  curves of Si nanowire devices with various illumination intensity, Inset: schematic diagram the device, (b) Photoresponsivity ( $\Delta I_d/I_{d0}$ ) change of Si nanowires FETs with different doping concentration by increasing light power intensity.

## Scanning Tunneling Microscopy and Spectroscopy of Novel Silver-Containing DNA Molecules

<u>Natalie Fardian Melamed</u><sup>†</sup>, Gennady Eidelshtein<sup>‡</sup>, Roman Zhuravel<sup>†</sup>, Dvir Rotem<sup>†</sup>, Alexander B. Kotlyar<sup>‡</sup>, and Danny Porath<sup>†\*</sup>

<sup>†</sup>Institute of Chemistry and Center for Nanoscience and Nanotechnology, The Hebrew University of Jerusalem

\* Corresponding author. E-mail: Danny.Porath@mail.huji.ac.il

<sup>‡</sup>Department of Biochemistry, Tel Aviv University

#### Abstract

The quest for a suitable molecule to pave the way to molecular nano-electronics has been met with obstacles for over a decade. Candidate molecules such as carbon nanotubes lack the appealing trait of self-assembly, while DNA lacks the desirable feature of conductivity. Silver-containing poly(G)-poly(C) DNA (E-DNA<sup>1</sup>) molecules were recently reported as promising candidates for molecular electronics, owing to the selectivity of their metallization, their uniform structure, their stability, their resistance to deformation, and their most possible conductivity. Here we present an elaborate temperature dependent high-resolution morphology characterization of these unique molecules, alongside a detailed depiction of their electronic level structure. Our findings were acquired by use of an ultra-high vacuum (UHV) scanning tunneling microscope (STM). The energy levels found for E-DNA indicate a novel, truly hybrid metal-molecule structure. These findings<sup>2</sup> add substantially to our knowledge about E-DNA molecules, leading to a further understanding of these molecules' conductive properties, bringing about their attractiveness as nanowires.

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## Centre for Analysis of Functional Materials (SAFMAT): Materials science and facilities

Jan Honolka<sup>1,\*</sup>

<sup>1</sup>Institute of Physics, AS CR, Prague, Czech Republic

The talk gives an overview on the research topics and experimental facilities at the EUsupported Center for Analysis of Functional Materials (**SAFMAT**) in Prague.

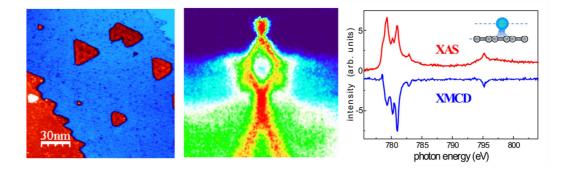
Founded in 2011, SAFMAT's installed facilities and experimental equipment is operated by laboratory staff in the user access mode for internal as well as external users, including services for industrial R&D (80% research, 10% student education, and 10% services for industry).

The SAFMAT laboratories focus on interdisciplinary research between physics, materials science, engineering and medicine. Examples of application-oriented research are shape memory alloys, multiferroics, as well as functional surfaces/coatings for medical devices and implants. On the other hand, more fundamental research in surface science is very active on 2D systems like graphene, topological insulators and molecular systems.

I will present a selection of recent research (see also link to *PragMat* group webpage below) on structural, electronic, and magnetic properties of 2D systems and Heusler alloys.

The potential of combining local *k*-space mapping (*Omicron NanoESCA*) with STM/AFM and EBSD techniques at SAFMAT is illustrated by the investigation of CVD-grown graphene monolayers on Cu-foils, where the vicinal surface morphology laterally modulates the graphene doping [1].

Ongoing research on other 2D materials are shortly reviewed, including topological insulators [2] and transition metal dichalcogenides, especially their interfaces with magnetic phases [3,4].



\* e-mail: honolka@fzu.cz, webpage: http://www.fzu.cz/~honolka/

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## **Chemistry on Graphene**

## Petr Kovaříček<sup>1</sup>, Zdenek Bastl<sup>1</sup>, Václav Vales<sup>1</sup>, Jana Vejpravova<sup>2</sup>, and <u>Martin Kalbac<sup>1</sup></u>

<sup>1</sup> J. Heyrovsky Institute of Physical Chemistry, CAS, Dolejškova 2155/3, 182 23 Prague, Czech Republic

<sup>2</sup> Institute of Physics, CAS, Na Slovance 2, 182 21 Prague, Czech Republic

Corresponding author: kalbac@jh-inst.cas.cz

The outstanding properties and potential of graphene are widely recognized in the scientific community. Covalent grafting of substituents to graphene is a promising way to tune the properties of this material. However, most of the approaches to functionalize graphene are based on reaction in liquid phase, which is not compatible with industrial needs. The novel result of this study therefore is the ability to perform covalent reactions, nucleophilic substitution, on pristine graphene by gas-phase methods.

The functionalized material was characterized by 'routine methods' including XPS, AFM and SEM. In addition we succeed to measure functional groups on single layer graphene directly using surface –enhanced Raman spectroscopy. Consequently, we could detect and confirm covalent grafting of the surface at a "single-molecule" level.

### Size-dependent charge transport in Au-seeded Ge nanowires

Maria Koleśnik-Gray

Lehrstuhl für Angewandte Physik, FAU Erlangen-Nuernberg, Staudstr. 7 Bau A3, Erlangen, Germany

Electrical transport properties of Au-seeded germanium nanowires were studied at ambient conditions as a function of their size. A non-trivial dependence of the electrical conductivity, mobility and carrier density on the nanowire radius was found. We show that while for nanowires with radius size above ca. 35 nm the chargecarrier drift is limited by electron-phonon scattering, in smaller radius nanowires ionized impurity scattering dominates. The results indicate that the electrostatic properties of thin (radius below 35 nm) nanowires are of quasi-one-dimensional character.

# Centre of functional materials for bio-applications (FUNBIO): aims and scope, instruments, results

Irena Kratochvílová<sup>1</sup>\*

<sup>1</sup>Institute of Physics, AS CR, Prague, Czech Republic

Centre of functional materials for bio-applications (FUNBIO) in the Institute of Physics AS CR (Operational Programme Prague Competitiveness structural funds of the European Commission) expand modern analytical methods for materials on the border between the organic and inorganic world used in advanced medical applications.

Instruments in the FUNBIO centre: scanning electron microscope, atomic force microscope for the organic materials surfaces, infrared spectral ellipsometer, optical lithography.

Nanodiamond particles adjusted for application in optically-traceable intracellular nanodiamond sensors -novel method for remote monitoring of chemical processes in biological environments Paper [1] Excellent Publications by Czech Council for Research, Development and Innovation [1,2], Liposomes as drug carriers in vaccine complexes. Synthetic vaccine against Lyme disease, Vaccine construct stability [3].

- Award of the Technological Agency of the Czech Republic 2015
- Award Cooperation of the Year 2014 (American Chamber of Commerce)
- Excellent GAČR project P304/10/1951 GA CR "Nanoliposomes for development of recombinant vaccines and targeted immunotherapeutics", 2014



e-mail: krat@fzu.cz, webpage: ofm.fzu.cz/irena-kratochvilova

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### **Electrical Characterization of 1D Molecular Structures**

<u>Avigail Stern<sup>1</sup></u>, Gideon I. Livshitz<sup>1</sup>, Dvir Rotem<sup>1</sup>, Suzanna Azoubel<sup>1</sup>, Shlomo Magdassi<sup>1</sup>, Genady Eidelshtein<sup>2</sup>, Alexander Kotlyar<sup>2</sup>, Danny Porath<sup>1</sup>\*

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

<sup>2</sup> Department of Biochemistry and Molecular Biology and the Center of Nanoscience and Nanotechnology, Tel Aviv University, Israel

\*Corresponding Author: Danny.Porath@mail.huji.ac.il

Charge transport through 1D polymers is intriguing, but extremely challenging to research. Detailed research of the mechanism of such transport has been detained, mainly due to shortage of reliable charge transport measurements through such molecules. In order to supply this shortage a reliable measurement setup, that is suitable for measurement of molecules tens to hundreds of nanometers long, is required.

Recently, a new measurement setup was developed in our lab that answers this requirement. This setup involves a stationary gold electrode that is evaporated over the molecules of interest and a conductive AFM tip serving as a second mobile electrode that contacts single molecules protruding from the gold electrode. We demonstrate the efficiency of this setup with two different types of 1D structures. The first is single-walled carbon nanotube junctions in a carbon nanotube network. For these structures we demonstrated the effect of HNO3 treatment on individual junctions, showing that the HNO3 improves the conductivity of each of the junctions. The second type of structure was gold coated DNA, for which we showed that the thicker the gold coating is, the longer the length of the molecule that is conductive.

## DNA origami nanostructures for application in nanoelectronics

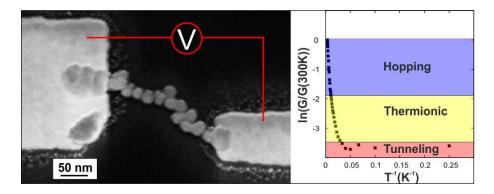
#### Bezu Teschome<sup>a,b</sup>, Stefan Facsko<sup>a</sup>, Tommy Schönherr<sup>a</sup>, Jochen Kerbusch<sup>a</sup>, René Hübner<sup>a</sup>, Kurt V. Gothelf<sup>c</sup>, Adrian Keller<sup>d</sup>, and Artur Erbe<sup>a</sup>

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

 <sup>b</sup>Technische Universität Dresden, Mommsenstraße 13, 01069 Dresden, Germany.
 <sup>c</sup>Danish National Research Foundation: Centre for DNA Nanotechnology (CDNA) at Interdisciplinary Nanoscience Center (iNANO) and Department of Chemistry, Aarhus University, 8000 Aarhus C, Denmark.
 <sup>d</sup>Technical and Macromolecular Chemistry, University of Paderborn, Warburger Str. 100, 33098

"Technical and Macromolecular Chemistry, University of Paderborn, Warburger Str. 100, 33098 Paderborn, Germany.

DNA origami [1] nanostructures are promising scaffolds for nanoelectronic [2] device fabrication due to their unique addressability which enables the site-selective modification with metallic and semiconducting nanoparticles, as well as their partial or complete metallization. In this work, we first demonstrate a compelling alternative approach to generate ordered arrays of DNA nanotubes on topographically patterned surfaces [3]. To this end, we combine two bottom-up techniques for nanostructure fabrication, i.e., DNA origami self-assembly and self-organized nanopattern formation on silicon surfaces during ion sputtering, thus avoiding the necessity of lithographic processing or chemical modifications. Then, we present the high-yield synthesis of high-density gold nanoparticle (AuNP) arrangements on DNA origami nanotubes with few unbound background nanoparticles and fabricate large arrays of aligned DNA origami nanotubes decorated with a high density of AuNPs [4]. The high yield of AuNP assembly was achieved by careful control of the buffer and the AuNPs concentrations and the hybridization time on Si surface. In addition, we optimize the metallization of DNA origami nanotubes to create DNA origami-templated nanowires and develop a platform for electrical contacting of those nanowires. Then, we measure the electrical conductance of the metallized nanowires at various temperatures from room temperature down to liquid helium temperature for two different nanowire morphologies. We also demonstrate the assembly of heterogeneous nanostructures on a single DNA origami nanotube.



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#### Magnetotransport properties of Mn-doped Bi<sub>2</sub>Se<sub>3</sub> topological insulator

<u>V. Tkáč</u><sup>1</sup>, V. Komanicky<sup>2</sup>, R. Tarasenko<sup>2</sup>, M. Vališka<sup>1</sup>, K. Carva<sup>1</sup>, P. Baláž<sup>1</sup>, P. Proschek<sup>1</sup>, V. Holý<sup>1</sup>, G. Springholz<sup>3</sup>, V. Sechovský<sup>1</sup> and J. Honolka<sup>4</sup>

<sup>1</sup>Department of Condensed Matter Physics, Faculty of Mathematics and Physics, Charles University, Ke Karlovu 5, CZ-12116 Prague 2, Czech Republic

<sup>2</sup>Institute of Physics, P. J. Šafárik University, Park Angelinum 9, 040 01 Košice, Slovak Republic <sup>3</sup>Institute of Semiconductor and Solid State Physics, Johannes Kepler University, Altenbergerstrasse 69, A-4040 Linz, Austria

<sup>4</sup>Institute of Physics, Academy of Sciences of the Czech Republic, Na Slovance 2, CZ-18221 Prague 8, Czech Republic

Three-dimensional (3D) topological insulators (TIs) are a newly discovered state of matter with insulating bulk and conducting topological surfaces states (TSSs). In prototype Bi-based chalcogenide TIs like Bi<sub>2</sub>Te<sub>3</sub> or Bi<sub>2</sub>Se<sub>3</sub>, a single spin-helical topological surface state (TSS) is generated by strong spin-orbit coupling, which is protected by time-reversal symmetry. 2D transport through TSS is predicted to be connected with the presence of weak antilocalization (WAL) effect. The gapless Dirac cone dispersion of the TSS carries a  $\pi$  Berry phase, which changes the interference of time-reversed scattering loops from constructive to destructive. This effect can be destroyed by applying a magnetic field, which breaks the  $\pi$  Berry phase, leading to a cusp-shaped negative magnetoconductivity.

Magnetic impurities violate time-reversal symmetry and thus may largely affect topological insulator properties and their transport. The mean field produced by magnetic doping may open a uniform gap at the Dirac point, allowing electrons to backscatter. Mn - induced gap at the Dirac point was observed using Angle-resolved photoemission spectroscopy (ARPES) in our samples [1]. The antiferromagnetic order was observed in the lowest temperatures in our previous magnetic studies [2]. The Curie temperature,  $T_{\rm C}$  roughly rises linearly between 4 and 6 K with increasing atomic concentrations  $x_{\rm Mn} \approx 0.06 - 0.14$  of manganese.

The present work is devoted to the study of Bi<sub>2</sub>Se<sub>3</sub> thin films with Mn dopants, which were grown by molecular beam epitaxy on insulating BaF<sub>2</sub> (111) substrates. We experimentally studied transport properties of the Mn-doped Bi<sub>2</sub>Se<sub>3</sub> topological insulators with various thickness and Mn concentrations. Bi<sub>2</sub>Se<sub>3</sub>-based Hall bars for transport measurements were fabricated using lithography techniques. The measurements of electrical resistivity, magnetoconductance and Hall resistivity have been realized at temperatures down to 0.3 K in magnetic fields up to 14 T in various orientations. At low temperatures we analyzed the electrical conductance using weak localization (WL) concepts for two dimensional systems and taking into account electronelectron interaction effects [3]. The presence of WAL effect was observed in the field dependence of the magnetoconductivity. The analysis of the WAL behavior using the Hikami-Larkin-Nagaoka formula correlates the phase coherence length and number of conductivity channels above and below the magnetic ordering temperature  $T_{\rm C}$ . Our findings manifest the direct consequences of the presence of a gaped TI surface state on the transport properties.

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Tailoring wrinkles in graphene by nanoparticles and fullerenes

J. Vejpravova<sup>\*1</sup>, B. Pacakova<sup>1</sup>, A. Mantlikova<sup>1</sup>, T. Verhagen<sup>1</sup>, V. Vales<sup>2</sup>, O. Frank<sup>2</sup> and M. Kalbac<sup>2</sup>

<sup>1</sup>Institute of Physics CAS, Na Slovance 2, Prague 8, Czech Republic <sup>2</sup>JH Institute of Physical Chemistry CAS, Dolejskova 3, Prague 8, Czech Republic

#### \*vejpravo@fzu.cz

We propose a general strategy for creation of a defined network of wrinkles in graphene. In order to take control over the wrinkling process, we engineered graphene - nanoparticle or graphene fullerene C<sub>70</sub> guasi two-dimensional structures [1, 2], constituted of isotopically-labelled graphene monolayers (grown by chemical vapour deposition) transferred over substrates decorated with the monodisperse nanoobjects acting as local sources of the graphene corrugation. The strain and doping in the model nanostructures were inspected by Raman spectro-microscopy, and their topography was evaluated by scanning electron microscopy and atomic force microscopy (AFM) [1-3]. Typical fingerprint of the wrinkles is identified as a substantial contribution to the principal Raman active modes (G and G'), which show dominant (G1, G'1) and red-shifted (G2, G'2) subbands [1,4]. The G-G' correlation analysis unambiguously assigned the G<sub>2</sub> and G'<sub>2</sub> components to the wrinkles. Finally, we put in context the results of the advanced AFM processing and Raman map analysis and obtained a general dependence of the amount of wrinkles on the relative intensity of the wrinklerelated subbands [1]. Our approach thus enables robust control over the graphene topography up to  $\sim 60\%$  of wrinkling and facile quantification of the wrinkling using Raman spectroscopy as the most convenient probe for the graphene. The customized wrinkle networks show ultimate exploitation in sensor design, controlled functionalization of graphene, (magneto)plasmon confinement and oriented cell growth.

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#### Towards electrical transport measurements through single DNA molecules

Roman Zhuravel, Haichao Huang, Haya Dachlika, Dvir Rotem and Danny Porath\*

Institute of Chemistry and The Harvey M. Krueger Center for Nanoscience and Nanotechnology, The Hebrew University of Jerusalem, Israel

The field of Nano-electronics concentrates a lot of interest from technological and scientific points of view. While charge transport in the solid state has been widely researched, for large single molecules many fundamental questions remain unsolved.

DNA is a good model molecule for many polymeric systems. Charge transport along DNA molecules has attracted scientific interest for over half a century. However, due to the many free parameters concerning these experiments, a variety of results were achieved, triggering an ongoing scientific debate on the DNA molecule conductivity. Our goal in this research is to reveal the charge transport mechanisms by controlled elucidation of the affecting parameters.

We create dimers of gold nanoparticles bridged by exactly one DNA molecule, where each nanoparticle is connected to the DNA trough one thiol. This system is very well-defined with a minimum number of unknown parameters. The dimer is brought to a small gap between pointing electrodes by dielectrophoresis for further electrical characterization. Our system enables precise source-drain-gate measurements with very good control of many environmental parameters such as temperature, surrounding ambience etc. These measurements have already generated promising preliminary results, which will be presented.

## NanoNet International Workshop 2016, Prague

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

### Calculating electron transport through aromatic and antiaromatic molecules.

<u>Narendra P. Arasu</u> and Héctor Vázquez Institute of Physics, Academy of Sciences of the Czech Republic Cukrovarnicka 10, Prague, Czech Republic

The conducting properties of single molecule circuits are strongly influenced by the chemical structure of the molecular backbone.  $\pi$ -conjugated systems are good conductors due to the delocalized nature of their molecular orbitals [1]. Recently the relationship between conductance and the degree of aromaticity of the molecule was investigated [2]. Here we address this question through first-principles simulations by comparing the conductance of an aromatic molecule to that of an antiaromatic one. The conjugated aromatic molecule is porphyrin, a class of molecules with potential applications in nanoscience and solar light harvesting [3]. We compare this to a norcorrole molecule having an antiaromatic core. Both molecules have a central Ni atom and are bonded through thioacetate linkers to Au. They are structurally similar, with the antiaromatic molecule having two fewer saturated C atoms than the porphyrin. We use Density Functional Theory (DFT) and Non-Equilibrium Green's Function (NEGF) methods to calculate electronic and transport properties of the molecular junctions, and apply a simple scheme to correct the position of DFT molecular levels [4]. We find that the molecular gap is smaller for the antiaromatic molecule than for the aromatic one. At the interface, conductance is LUMO-dominated in both cases. However, the position of the antiaromatic LUMO resonance is closer to the Fermi level than in the aromatic case, which makes the antiaromatic complex ~20× more conducting than the aromatic one. Our study thus contributes to a new avenue in single molecule junction studies.

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# Stacking different two-dimensional materials to fabricate a high mobility transistor

<u>H. Arora<sup>1,2</sup></u>, G. Seifert<sup>3</sup>, G. Cuniberti<sup>4</sup>, M. Helm<sup>1,2</sup>, A. Erbe<sup>1</sup>

<sup>1</sup>Helmholtz-Zentrum Dresden Rossendorf, Bautzner Landstrasse 400, 01328 Dresden <sup>2</sup>Technical University Dresden, Faculty of Mathematics and Natural Sciences, 01062 Dresden <sup>3</sup>Technical University Dresden, Institute for Physical Chemistry and Electrochemistry, 01062 Dresden

<sup>4</sup>Technical University Dresden, Institute for Materials Science and Max Bergmann Centre of Biomaterials, 01062 Dresden

Two-dimensional (2D) materials have gained enormous attention in recent years owing to their excellent transport properties and mechanical flexibility. Several two-dimensional (2D) semiconducting materials like graphene, MoS<sub>2</sub>, WSe<sub>2</sub>, silicene, germanene, phosphorene have been produced and intensively studied. Their semiconducting properties allow the development of 2D structures, whose electronic properties can be tuned. Another exciting frontier in the field of 2D materials which has opened up new opportunities is stacking them together. Different 2D materials are combined in such a way that all their different advantages can be properly utilized to achieve the desired application.

In this project, the aim is – to investigate novel 2D nanostructures and materials, and to stack them together to fabricate heterostructures, followed by their structural and electrical characterization. The first series of experiments were carried out with porphyrin-based 2D polymers and mechanically exfoliated  $MoS_2$  flakes. A highly sophisticated contacting scheme was developed to contact them using electron-beam lithography (EBL), followed by their electrical characterization. Currently, the contacting and characterizing schemes optimized on these materials are being transferred to other novel 2D materials. In future, the aim will be to fabricate a heterostructure by stacking different 2D materials, whose different properties can complement each other to fabricate a transistor.

## Electrical Transport Properties of Two dimensional CVD grown Molybdenum disulfide (MoS<sub>2</sub>)

Wajid Awan<sup>1</sup>, Tommy Schönherr<sup>1</sup>, Stefan Facsko<sup>1</sup>, Xinliang Feng<sup>2</sup>, Artur Erbe<sup>1</sup>

<sup>1</sup>Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany <sup>2</sup>Technische Universität Dresden, 01069 Dresden, Germany

Transition metal dichalcogenides came into the picture and got a place in a wide range of novel applications as well as in basic research. Strikingly,  $MoS_2$  receives significant attention since it undergoes transition from indirect bandgap (bulk form) to a direct bandgap (1.2eV) semiconductor if thinned out to a single atomic layer. The bandgap is an essential property for tunable 2-D nanodevices. We performed electrical transport measurements at room temperature for CVD grown  $MoS_2$  on  $SiO_2/Si$  substrate. Standard Electron beam lithography (EBL) was used to pattern Gold (Au) metal contacts on  $MoS_2$  flakes. For the purpose of sample characterization, we performed the Atomic Force Microscopy (AFM) and Raman Spectroscopy techniques, respectively, which confirm that the thickness of the CVD grown  $MoS_2$  triangular flakes corresponds to single layers. Low temperature characterization of the electrical properties of the layers elucidates the exact mechanisms of charge transport in the 2d-layers. This knowledge will be used to modify the electrical properties in a controlled way, for example by ion irradiation.

Email: a.awan@hzdr.de

## Structural, Optical and Electrical Characteristics of BaSrTiO<sub>x</sub>Thin Films Deposited by RF Magnetron Sputtering

Turkan Bayrak<sup>1</sup>, Necmi Biyikli<sup>1,2</sup>, Eda Goldenberg<sup>1</sup>

<sup>1</sup>National Nanotechnology Research Center (UNAM), Bilkent University, Bilkent, Ankara 06800, Turkey <sup>2</sup>Institute of Materials Science and Nanotechnology, Bilkent University, Bilkent, Ankara 06800, Turkey Corresponding author: t.bayrak@hzdr.de

ABO<sub>3</sub>-type perovskite oxides, where A and B denote two different cations, have recently attracted a great interest for their potentials in oxide-based electronics, because of their multifunctional opto-electronic properties including their high optical band gap and dielectric constants. Among several perovskite thin films BaSrTiO<sub>3</sub> (BST) thin films are key elements for the development of high performance electronic devices, and their reliability and efficiency depend strongly on the precise knowledge of microstructure, as well as optical and electrical constants. In the present work, we have deposited BaSrTiO<sub>x</sub> films with rf magnetron sputtering technique at room temperature on UV fused silica and Si substrates. The dependences of film microstructure, surface morphology, absorption edge, refractive index, and dielectric constants on deposition pressure, partial oxygen flow and the postdeposition annealing were examined by grazing-incidence X-ray diffraction (GIXRD), scanning electron microscopy (SEM), spectrophotometry, ellipsometry, as well as photoluminescence, capacitancevoltage and current-voltage measurements. For all as-deposited films, the average optical transmission was ~85% in the visible and near infrared spectrum. Metal-insulator-semiconductor (Ag/BST/p-Si) diodes were fabricated and characterized by capacitance-voltage and current-voltage measurements. Initial results revealed that low-temperature-grown BST thin films have promising properties for device applications.

### STM study of activated fullerene – Au(111) coupling

#### T. Chutora<sup>a</sup>, J. Redondo<sup>a</sup>, H.Vazquez<sup>a</sup>, M. Svec<sup>a</sup> and P. Jelinek<sup>a</sup>.

<sup>a</sup>Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic

Molecular self-assembly on surfaces has attracted a great deal of attention during the past decade, because of its potential in molecular electronic device fabrication [1]. The coupling of molecules to the metal surfaces determines its electronic properties. The understanding of their electronic properties is the first step towards designing functional electronic devices. Fullerenes on metal surfaces are among the most extensively studied systems. Due to their very practical properties, fullerenes are a key topic of nanotechnology and industrial research also nowadays. Here we study a new type of system: fullerenes with artificially created defects, which bind to Au(111) surface via covalent bonds. These bonds were shown to be highly-conducting and stable [2,3].

First, we deposited  $C_{60}$  on the clean Au(111) substrate. The molecule formed self-assembled islands as expected. In the next step, we use the Ar<sup>+</sup> ions to successfully remove C atoms from the  $C_{60}$  molecules. Defects inside the  $C_{60}$  islands formed by sputtering were distinguished and characterised by atomically resolved STM. We can also clearly observe single molecules which were detached from the islands as the result of the sputtering process. These functionalized molecules bind to the kinks in the herringbone reconstruction of the substrate.

Density-Functional theory calculations reveal the electronic structure at the interface. The unsaturated C atoms exposed by the Ar<sup>+</sup> sputtering react with the Au surface. Different binding geometries are studied and their electronic and spectroscopic properties are calculated.

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### Top-down fabrication and characterization of reconfigurable silicon nanowirebased field effect transistors

<u>Dipjyoti Deb</u><sup>1, 2,3</sup>, Muhammad Bilal Khan<sup>1</sup>, Yordan M. Georgiev<sup>1,2,3</sup>, Markus Löffler<sup>3</sup>, Walter Weber<sup>2,3</sup>, Manfred Helm<sup>1,2,3</sup>, and Artur Erbe<sup>1,2,3</sup>

<sup>1</sup>Institute of Ion Beam Physics and Materials Research, HZDR, Dresden, Germany <sup>2</sup>International Helmholtz Research School for Nanoelectronic Network, HZDR, Dresden, Germany <sup>3</sup>Center for Advancing Electronics Dresden, TU Dresden, Dresden, Germany, Author: d.deb@hzdr.de

In the last 60 years the size of a transistor has been reduced from few centimeters to few nanometers. Smarter, faster and cheaper: these are the three factors that motivated the miniaturization crusade in the silicon chip industry. Now we reach the end of physical scaling and it is expected that future development will be based on new ideas [1] : (i) new materials (high-mobility channel materials accompanied by metal gates with high-k gate dielectrics), (ii) new architectures (e.g. 3D integration), (iii) new functionality (e.g. reconfigurability), (iv) new computation principles (e.g. spintronics, quantum computing), etc.

In this work we deal with this problem by introducing reconfigurability in transistors. We report on characterization of reconfigurable, undoped silicon nanowire field effect transistors (FETs) with Schottky junctions fabricated on silicon on insulator (SOI) substrates by an industry compatible top-down process. Reconfigurable transistors employ an axial nanowire heterostructure (metal/intrinsic-silicon/metal) with independent gating of the two Schottky junctions and can be reversely configured as p-FET or n-FET simply by the application of an electric signal [2].

The fabrication scheme is based on electron beam lithography (EBL) using hydrogen silsesquioxane (HSQ), a negative-tone electron beam resist, followed by inductively-coupled plasma (ICP) etching. The etch recipe was optimized with respect to selectivity, sidewall roughness and anisotropy by selecting an appropriate gas chemistry ( $SF_6/C_4F_8$ ) and controlling the ICP hardware parameters such as gas flow, mixed gas ratio, plasma power and chamber pressure. We produced silicon nanowires of 20 nm width and nanowire arrays with a pitch of  $\approx$  200 nm.

A nickel (Ni) layer of 50 nm thickness was sputtered on the Si nanowires at lithographically defined areas followed by lift-off and thermal annealing to create nickel-silicide Schottky junctions inside the nanowires. In this way, the source and drain regions were formed creating silicide-silicon-silicide contacts. Diffusion of Ni in Si nanowires was precisely controlled by the radial crystal orientation of the nanowires, which was checked by transmission electron microscopy (TEM). The Schottky junctions were electrostatically modulated by a back gate potential. Transport properties of these nanowires could be switched from p-type to n-type and vice-versa by changing the polarity of the back gate.

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### Physical growth of metallic helix arrays on substrates with different thermal properties

#### Günter Ellrott

#### Abstract

Free-standing and vertically aligned metallic nanohelical structures can be produced using glancing angle deposition on nanodot-patterned substrates via electron beam evaporation. During the physical growth, the structure of the helices is strongly affected on the substrate temperature, therefore adequate control over the temperature is crucial. Since standard evaporation chambers do not allow for active cooling of a rotating sample, another approach has been developed.

We demonstrate that by using a combination of a high-thermal conductivity material (e.g. silicon carbide) with different low thermally conducting metal layers on top it is possible to grow helices at room temperature without the need for active cooling. This method allows for direct contacting of the nanohelix arrays into electronic devices. Furthermore, silicon carbide is transparent for the visible spectrum, making it an ideal support for optical characterization of the helices.

### Magnetism and superconductivity of 2D FeSe layers grown on Bi<sub>2</sub>Se<sub>3</sub> topological insulators

J. Fikáček<sup>1</sup>, M. Vondráček<sup>1</sup>, V. Holý<sup>2</sup>, G. Springholz<sup>3</sup> and J. Honolka<sup>1</sup>

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

<sup>2</sup> Department of Condensed Matter Physics, Faculty of Mathematics and Physics, Charles University in Prague, 120 00 Prague 2, the Czech Republic

<sup>3</sup> Johannes Kepler University Linz, Institute of Semiconductor and Solid State Physics, Altenbergerstrasse 69, A-4040 Linz, Austria

Bulk FeSe is a thoroughly studied member of chalcogenide superconductors. Its plain cubic structure simplifies theory calculations and thus makes it an interesting superconductor model system. The critical temperature for superconductivity can be appreciably tuned by external pressure, element substitution or carrier doping.

In recent years, several studies were focused on FeSe films grown on different substrates. Among others a study devoted to FeSe monolayers grown on  $SrTiO_3$  revealed a tremendously enhanced  $T_c$  above 100 K, which looks very promising for future applications [1]. Surprisingly, adding more FeSe monolayers suppresses the superconducting state contrary to FeSe on top of a bilayered graphene (0001) substrate where  $T_c$  scales with the number of FeSe layers towards the value observed for bulk FeSe (~ 9 K) [2]. The former suggests that superconductivity in FeSe is not just driven by pressure/strain, but also by interface effects. Moreover, a stoichiometry towards a slightly Fe-rich phase seems to be important.

We will present our plans for future measurements on an ongoing research of FeSe grown by molecular beam epitaxy (MBE) on a  $Bi_2Se_3$  matrix. First results showed that FeSe is not superconducting down to 6.5 K [3]. Adding a superconducting material on top of a topological insulator may bring new interesting phenomena at the interface due to proximity effects, where topological surface states interact with superconducting states of FeSe. In particular it will be interesting to study why similar heterostructures  $Bi_2Te_3$ /FeTe [4] and FeTe/Bi\_2Te\_3 [5] both exhibit superconductivity although neither  $Bi_2Te_3$  nor FeTe is superconducting in the bulk.

Sample qualities will be checked by LEED and STM techniques. Further characterization via XPS and ARPES will be done using a NanoESCA instrument at the SAFMAT in Prague. Magnetic properties of  $Fe_{1+x}Se_{1-x}$  samples can be probed in a variable temperature MOKE instrument (T = 3K -380K, magnetic fields either in plane or in the perpendicular direction). The instrument is equipped with a magneto-transport option, which allows to directly correlate the formation of magnetic and superconducting phases.

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Keywords: superconductivity, topological insulators, layered structures.

#### Towards an Electronic Model for Reconfigurable Transistors

<u>Florian Fuchs</u><sup>1,2</sup> (f.fuchs@hzdr.de), Jörg Schuster<sup>2,3</sup>, and Sibylle Gemming<sup>1,2</sup>

<sup>1</sup>Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany <sup>2</sup>Center for Advancing Electronics Dresden, Dresden, Germany <sup>3</sup>Fraunhofer Institute for Electronic Nano Systems, Chemnitz, Germany

In contrast to conventional CMOS transistors, reconfigurable field effect transistors (RFETs) can be switched between n- and p-type behavior, which allows more compact and flexible circuit designs [1, 2]. Symmetry between n- and p-current is required and this can be achieved by strain engineering as experimentally demonstrated in Ref. [2]. However, a detailed understanding of the electron transport across the strained interface is not yet available and requires electronic models to capture all relevant transport mechanism.

We investigate the relation between strain and electron transport properties of planar interfaces between metallic NiSi<sub>2</sub> and semiconducting Si in  $\langle 110 \rangle$  crystal orientation. We apply the non-equilibrium Green's functions formalism together with density functional theory as implemented in Atomistix ToolKit [3] to calculate the transmission spectra. Using a modified version of the Landauer formula, we than obtain an expression for the current through the RFET and hence, the transfer characteristic can be investigated.

Fig. 1 (left) shows a comparison between the calculated transfer characteristic using this model and experimental reference data [2]. A very good agreement can be seen which verifies our model. However, in the experiment, the RFET was compressed during the oxidation process. Because the structure in the simulation was supposed to be unstrained, some pre-strain might be present in the simulation. We also study how strain, either applied perpendicular or parallel to the transport direction, alters the current. An example is given in Fig. 1 (right) for perpendicular strain. It can be seen that a small amount of strain is sufficient to change the ratio between n- and p-current and that symmetry can be achieved. Considering the above-mentioned pre-strain in the simulation, the general trend is also in agreement with experimental studies [1, 2].

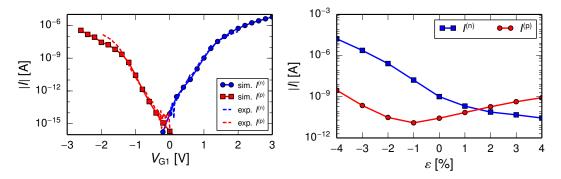


Figure 1: Left: Simulated RFET characteristics and experimental results from Ref. [2]. Right: Simulated current at  $V_{G1} = \pm 1$  V for different strain perpendicular to the transport direction.

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# Chemical doping of semiconducting donor-acceptor polymers: a DFT study of the charge transfer

<u>Florian Günther</u>,<sup>a,b</sup> Anton Kiriy,<sup>c</sup> Sibylle Gemming,<sup>a,d</sup> and Gotthard Seifert<sup>b</sup>

<sup>a</sup> Helmholtz-Zentrum Dresden-Rossendorf, Center for advancing Electronics Dresden (cfaed), Germany. Email: f.guenther@hzdr.de

<sup>b</sup> Institute of Physical Chemistry and Electrochemistry, University of Technology Dresden, Center for advancing Electronics Dresden (cfaed), Germany.

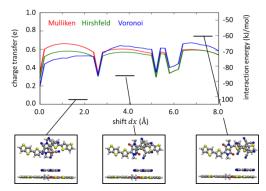
<sup>c</sup> Leibniz-Institut für Polymerforschung Dresden Center for advancing Electronics Dresden (cfaed), Germany. <sup>d</sup>Institute of Physics, Technical University Chemnitz, Germany.

#### Abstract:

[3]-Radialene-based dopant hexacyano-trimethylenecyclopropane (CN6-CP) had been found to be the strongest molecular p-dopant reported in open literature so far. Films of poly-Diketopyrrolopyrrole-dithienylthieno[3,2-b]thiophene (pDPP-TT) doped by CN6-CP exhibit electrical conductivities up to 50 S/cm which is one of the highest conductivity for molecularly doped semiconducting polymers [1].

In this study, we theoretically evaluate the doping effect of pDPP-TT models and CN6-CP or further pdopant molecules such as tetrafluorotetracyanoquinodimethane (F4-TCNQ) based on density functional theory (DFT) calculations. For this aim, we consider HOMO-LUMO gap opening, wave function hybridization, and charge transfer in terms of population analysis. Different structural complex formations are under consideration to evaluate the yield of doping and the stability when the dopant is located on different parts of the polymer. Interestingly, we observe in the lowest energy complex, the dopant molecule is located quite closely to the acceptor unit of the polymer (DPP) where the charge transfer process proceeds to the lowest extend.

To confirm the obtained theoretical results, we compare to experimental data such as UV-vis-IR spectroscopy studies.



Calculated charge transfer and energy for a CN6-CP:TT-DPP-TT charge transfer complex model. The shift indicates the relative distance of the centers of masses of the two molecules in the backbone direction. The colored curves specify the charge transfer obtained by the different population analyses (left scale) while the black bars show energies of the 6CN-CP:TT-DPP-TT complex relative to the individual molecules (right scale).

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### Aging Universality Classes in Surface Growth Models

Jeffrey Kelling<sup>1,2</sup>, Géza Ódor<sup>3</sup>, Sibylle Gemming<sup>1,4</sup>

 <sup>1</sup>Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Germany
 <sup>2</sup>Department of Information Services and Computing, Helmholtz-Zentrum Dresden-Rossendorf, Germany
 <sup>3</sup>Institute of Technical Physics and Materials Science, Hungarian Academy of Sciences, Budapest, Hungary
 <sup>4</sup>Institute of Physics, TU Chemnitz, Germany

Corresponding author: j.kelling@hzdr.de

Extensive dynamical simulations of a 2 dimensional driven dimer lattice gas are presented, which can be mapped to (2+1) dimensional surface growth in the Kardar-Parisi-Zhang (KPZ) or Edwards-Wilkinson (EW) universality classes. From this autocorrelation functions have been determined for the KPZ and EW universality classes and the underlying lattice gas. Studying the effects of different dimer lattice gas dynamics revealed strong differences in the aging behavior of the stochastic cellular automaton (SCA) and the random sequential update models. We show numerical evidence for nontrivial corrections as well as different universal scaling behaviors.

# Fabrication of sub-20 nm silicon nanowires using inductively coupled plasma etching

Muhammad Bilal Khan, Dipjyoti Deb, Yordan M. Georgiev, and Artur Erbe

#### Helmoltz Zentrum Dresden Rossendorf

Development of etching process for fabrication of ultrathin silicon nanowires (SiNWs) with inductively coupled plasma (ICP) source and C<sub>4</sub>F<sub>8</sub>/SF<sub>6</sub> mixed gas recipe at 18  $^{0}$ C is reported. Etch selectivity of silicon (SOI) to hydrogen silsesquioxane (HSQ), a negative tone electron beam resist and selectivity of silicon (SOI) to SiO<sub>2</sub> are investigated to identify suitable process window. Effects of ICP power, RF power, chamber pressure, flow rates and ratio of C<sub>4</sub>F<sub>8</sub>/SF<sub>6</sub> on etch rate, selectivity and surface roughness are examined. Atomic force microscopy (AFM) is used for identifying surface roughness of the silicon (SOI) substrates after etching. Thereafter, etching of patterned substrates is performed. Scanning electron microscopy is performed to observe the etch profile. Parameters such as flow rates of C<sub>4</sub>F<sub>8</sub>/SF<sub>6</sub> are optimized to attain sub-20 nm SiNWs with smooth and vertical sidewall.

### Single Level Molecule Measurement

Filip Kilibarda<sup>1</sup>, Omair Ahmed<sup>1</sup>, Gözde Öktem<sup>2</sup>, Anton Kiriy<sup>2</sup>, Artur Erbe<sup>1</sup>

<sup>1</sup> Institute of Ion Beam Physics and Materials Science, Helmholtz-Zentrum Dresden – Rossendorf, Dresden, Germany
<sup>2</sup> Leibniz-Institut f
ür Polymerforschung Dresden e.V. (IPF), Dresden, Germany

Corresponding author: f.kilibarda@hzdr.de

In recent years, microelectronics industry is reaching its limits with transistor miniaturization. One of the possibilities is to abandon standard silicon technologies and start using single molecules and atoms as building blocks. By taking this route, it is first important to characterize and choose the right molecular candidates for future implementation. Till recent years, this area was very slow in development, but as the techniques of electronic lithography, nanoscale manufacture and chemical synthesis continue to improve, it is accelerating in progress. In our research, we are working with Mechanically Controlled Break Junctions (MCBJ) as a method of characterizing electrical properties of molecules and apply Landauer theoretical approach to model the behavior of the junctions. In parallel to that, we are examining possibilities to gate the molecules while they are being characterized. Our experiments show successful coupling to the molecules and the accompanying change in conductance. In regard to gating, we show possibility of manufacturing sub-15nm gaps for side gating of the molecular system. The developed techniques presented here may prove to be important in future many-level measurements and transistor implementation.

**Domain walls in SrMnO3 thin films under epitaxial tensile strain** — •LOKAMANI <u>LOKAMANI</u><sup>1</sup>, CARINA FABER<sup>3</sup>, PETER ZAHN<sup>1</sup>, NICOLA SPALDIN<sup>3</sup>, and SIBYLLE GEMMING<sup>1,2</sup> — <sup>1</sup>Institute of Ion Beam Physics and Materials Research, HZDR e.V., 01314 Dresden, Germany — <sup>2</sup>Institute of Physics, Technische Universität, 09107 Chemnitz, Germany — <sup>3</sup>Materials Theory, ETH, 8093 Zürich, Switzerland

Strontium manganate (SrMnO<sub>3</sub>), a perovskite polymorph, exhibits cubic structure at low temperatures, which transforms into a hexagonal one at high temperatures. Density-functional calculations showed earlier, that under tensile strain the ground state of bulk SrMnO3 corresponds to a G-type-antiferromagnetic (G-AFM) cubic structure. If deposited as epitaxially strained thin film a rearrangement of the MnO<sub>6</sub> coordination polyhedra was calculated, which is antiferrodistortive in the plane parallel to the substrate[1]. Recently, ferroelectric domains have been observed experimentally in thin films of SrMnO<sub>3</sub> (20nm) on (001)-oriented LSAT with a 1.7% tensile strain[2]. Strikingly, the domain walls were found to be electrically insulating, rendering the domains to form stable nano-capacitor.

Here, we present a first-principle investigation of the domain wall formation in thin films of  $SrMnO_3$ , their non-conductive behaviour and the effect of vacancies and defects on the conductance properties of such domain walls.

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### Growth of Epitaxial Graphene on 6H-SiC(0001) in Ar Atmosphere

Jesús Rubén López Redondo<sup>1</sup>

<sup>1</sup> Thin Surfaces and Nanostructures, FZU, Prague, Czech Republic

Corresponding author: ruben@fzu.cz

Thermal decomposition of SiC wafers was proven to be a reliable method to obtain Epitaxial Graphene. Usually, the sublimation of Si induced by annealing of SiC substrates is difficult to control and hence a mix of buffer layer, singleand bilayer graphene is created, with rather high density of atomic steps. Therefore, the main challenge is to develop a method of making singlelayer graphene on a largest possible portion of the substrate. Thus, we devised a compact chamber for the graphene growth in Ar atmosphere, that can achieve desired parameters with minimal requirements. We study the process of graphene growth on the SiC(0001) substrates and get homogeneous singlelayer graphene overlayers spanning over micrometersized terraces.

# Enhanced stability of few-layer black phosphorus capped with TCNQ layer

Laura Meingast<sup>1</sup>

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

Corresponding author: I.meingast@gmx.net

The 2D layered semiconducting material black phosphorus attracts interest as a potential electronic and electrochemical device component. However, the application of black phosphorus into functional devices is inhibited by the fast degradation of the material under exposure to air. In the case of pristine black phosphorus exposed to ambient conditions, we observe a rapid formation of phosphoric-acid 'bubbles' at the surface which increase in size with time. In order to suppress this effect, we deposited a thin layer of TCNQ on top of mechanically exfoliated few-layer black phosphorus. AFM imaging revealed an increased stability over an extended period of time of the TCNQ-passivated layers.

#### Theoretical modeling of Persulfurated Coronene molecules on Au(111)

Seddigheh Nikipar, Dmitry Skidin, Dmitry Ryndyk, Francesca Moresco, Gianaurelio Cuniberti

Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, 01069 Dresden, Germany

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

Nowadays novel electronic devices based on single organic molecules are suggested as an alternative to inorganic semiconductor devices, this motivates the investigation of organic molecules and 2D molecular materials on different surfaces. In particular, carbon-sulfur compounds, such as  $C_{16}S_8$ , known as "sulflower", were investigated, being the first example of heterocyclic circular molecules. Recently, the new generation of sulflower components has been synthesized in the group of Prof. Xinliang Feng at TU Dresden, which is a fully sulfur-terminated polycyclic aromatic hydrocarbon molecule called persulfurated coronene (PSC,  $C_{24}S_{12}$ ).

Experimentally, PSC molecules were deposited on the gold surface under vacuum conditions. To investigate the molecular geometry and electronic structure, STM imaging and spectroscopy was used. In parallel, the theoretical simulations have been performed to support the experimental results and provide further insight into the physical and chemical properties of this novel molecule on metal surfaces. We present the atomistic simulations based on the density functional theory (DFT) and combined it with the Tersoff-Hamann approach to calculate the STM current-voltage curves, as well as the STM topography images, electron density of states and dI/dV curves. The outcome shows the reasonable agreement with the experimental results.

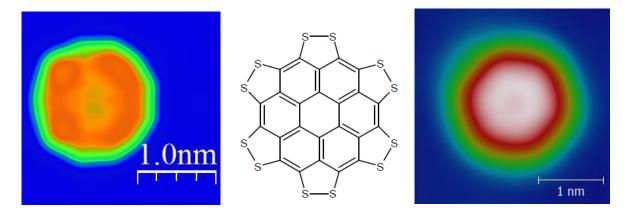


Figure: the structure of isolated PSC (center), the topography images of PSC molecule on Au(111) surface, image sizes: 3nm x 3nm, bias: 0.1 V, the theoretical calculation (left) and the experimental result (right).

# One step forward: Oligo(3-hexylthiophene) wires decorated with donor-acceptor chromophores

<u>Gözde Öktem</u><sup>1,2,3</sup>, Rainer Jordan<sup>2,3</sup>, Anton Kiriy<sup>1,3</sup>

<sup>1</sup>Leibniz-Institut für Polymerforschung Dresden e.V., Dresden, Germany <sup>2</sup>Professur für Makromolekulare Chemie, Technische Universität Dresden, Germany <sup>3</sup> International Helmholtz Research School for Nanoelectronic Networks, Dresden, Germany

Corresponding author: <a href="mailto:oektem@ipfdd.de">oektem@ipfdd.de</a>

A series of double-end functionalized, fully conjugated oligo(3-hexylthiophene)s modified with donor-acceptor (D-A) moleties, namely dimethylaniline-tetracyanobutadiene (DMA-TCBD), ferrocene-tetracyanobutadiene (Fc-TCBD) are synthesized. N,N-dialkylaniline and ferrocene derivatives are served as good activators for a strong electron donor alkyne used in the formation of main/side chain D-A type conjugated oligomers via click chemistry type postfunctionalization.<sup>1</sup> The alteration of oligomeric backbone with DA substitutions is provided by both in-situ modifications during polymerization and post-modifications after polymerization to incorporate chromophores into the structure as both end and pendant groups, respectively. Kumada catalyst-transfer polymerization (KCTP) is used to obtain oligo(3-hexylthiophene) wires with D-A anchoring groups by the termination of polymerization with highly electron rich alkynes and the conversion of that alkyne functionality to donor-substituted tetracyanobutadiene chromophores by the addition of electron-deficient ethene moieties. The latter one, D-A chromophores positioned at the oligomer side chains, deals with the postfunctionalization of regioregular oligo(3-hexylthiophene)s from KCTP by a three-step highyielding route sequentially consisting of the creation of an active site, insertion of highly electron-rich alkynes and click-postfunctionalization for the formation of TCBD functionality.<sup>2</sup> These smooth alterations at the end & pendant positions enable fine-tuning of optical/electronic energy band gaps and lowest unoccupied molecular orbital (LUMO) energy levels owing to change in electronic nature of oligomeric backbone. The redox properties in both anodic and cathodic directions are examined by cyclic voltammetry and HOMO-LUMO energy levels are determined accordingly. The quantitative click-type postfunctionalization at side chains is confirmed by the comprehensive analyses with NMR, MALDI-TOF. Additionally, the effect of incorporation traceable D-A units in conjugated systems as well as increase in the guantity of D-A units per oligomer chain on optical and electrochemical properties is analyzed. The implementation of KCTP and post-polymerization modification for the generation of functionally tunable donor-acceptor units in a finite number per oligomer chain is investigated in terms of charge transport properties.

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#### Low- temperature atomic force microscopy of wrinkled graphene

B. Pacakova, T. Verhagen, Z. Kominkova, M. Kalbac, J. Vejpravova

We present here a method of direct measurement of thermal expansion of water/ice beneath the GN layer. We demonstrate the method on the homogeneously wrinkled GN sheet, with the fine GN wrinkles filled with the water. So far, only few experimental data of the water ice thermal expansion are available since 1899, mostly based on the dilatometry, density measurement, interferometry or synchrotron x-ray diffraction.

Our approach is based on the low-temperature atomic force microscopy (AFM) measured down to 10 K. AFM serves as the direct probe of thermal expansion of system, analysing the topography of the GN wrinkles captured at different temperatures in the temperature range of 10 - 300 K. We observed global decrease of the wrinkle height,  $h_{WR}$  with decreasing temperature, followed by increase from 50 K to 10 K, qualitatively corresponding with evolution of the low-temperature ice expansivity. Results are supported by the room temperature IR spectroscopy measurement and low-temperature Raman spectroscopy data. Our data suggest that the thermal expansion of our system becomes negative around 74 K.

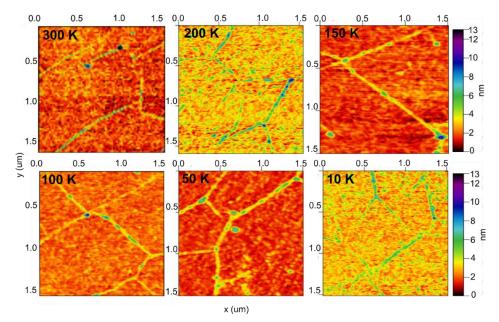


FIGURE 1. The topography AFM image of wrinkled GN measured at different temperatures in temperature range 10 - 300 K.

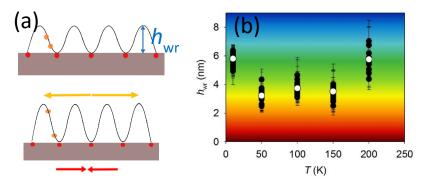


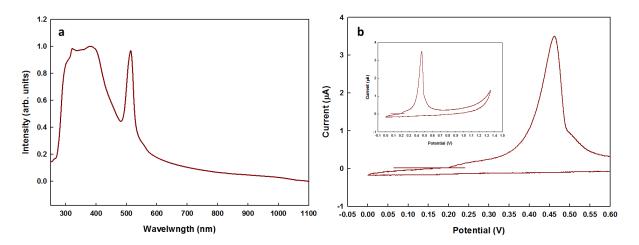
FIGURE 2. (a) Schematics of the wrinkled GN bellow and after cooling.  $h_{WR}$  as the wrinkle height. (b) Temperature dependence of  $h_{wr}$  in colouring of the AFM topography images.

## Two dimensional Perovskites: Morphological and Optoelectronic Characterizations

P.Goutham Raj<sup>1,2,3</sup>, Prof. Dr. Brigitte Voit<sup>1,2,3</sup>, Dr. Anton Kiriy<sup>2,3</sup>.

<sup>1</sup>Technische Universität Dresden, Germany, <sup>2</sup>Leibniz-Institut für Polymerforschung Dresden e.V. Germany, <sup>3</sup>IHRS NANONET.

Three-dimensional organic-inorganic hybrid perovskites have emerged as promising photo absorber material. Recently perovskite solar cells have exhibited efficiency as high as  $20\%^{1}$ . Despite of high in efficiency, 3D perovskite solar cells have poor environmental stability. In contrast, the lower dimension perovskites, 2D perovskite have shown excellent stability, but poor efficiency. To move from the 3D to the 2D perovskites, the small Methyl ammonium MA<sup>+</sup> cation is replaced by a much bulkier organic primary ammonium cation, thus confining the perovskite in two dimensions because of steric effects. We report the synthesis, morphological and optoelectronic characterizations of 2D perovskite thin films ((C<sub>4</sub>H<sub>9</sub>NH<sub>3</sub>)<sub>2</sub>PbI<sub>4</sub>). The morphologies revealed under scanning electron microscopy and atom force microscopy show well defined array of perovskite crystals with sizes of few microns and crystals having nearly flat surface with small roughness. Higher optical band gap of 2.21 eV was obtained for 2D perovskite (C<sub>4</sub>H<sub>9</sub>NH<sub>3</sub>)<sub>2</sub>PbI<sub>4</sub> thin films compared to 3D perovskite films, which is in agreement with literature. HOMO level of -5.30 eV was identified from the perovskite thin film using cyclic voltammetry.



Fugure 1: (a) UV-Visible absorption spectroscopy and (b) cyclic voltammetry of 2D perovskite thin film

#### Fabrication and Microfluidic Integration of Nanoscaled Sensor Elements

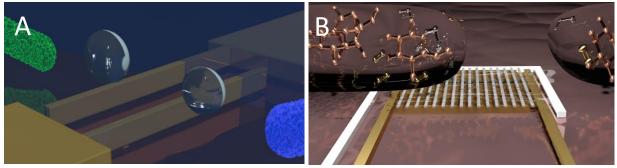
Julian Schütt<sup>1</sup>, Larysa Baraban<sup>1</sup>, Gianaurelio Cuniberti<sup>1</sup>

<sup>1</sup>Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, Budapester Str. 27, 01062 Dresden, Germany Corresponding author: <u>julian.schuett@nano.tu-dresden.de</u>

Detection of pathogens at low concentrations and sample volumes is one of the mainstreams in the current biomedical research due to the distinct demographic changes and wide spreading of the chronic and severe illnesses. Conventional pathogen detection approaches like flow cytometry, real time polymerase chain reaction and microarrays require high sample volumes, trained personnel, long detection times and bulky and expensive equipment. Consequently, there is a high demand for precise, cheap and portable sensor devices for application in the environment where the patient needs a proper treatment without available qualified personnel and hospitals, *e.g.* in developing countries.

In the first part, we faced the challenge to establish a MEMS-sensor capable of single cell detection based on dynamic impedance analysis using gold nanowires (See figure 1, panel A) to overcome the aforementioned limitations. The detection of cells one by one is realized in flow, employing the cytometry principle. The transport system consists of a 3D focusing microfluidic structure, which converts the analyte solution between the top-down fabricated gold nanowires, allowing higher sensitivity and selectivity due to electric field enhancement at the nanowire tips as well as higher signal-to-noise ratio by ballistic electron transport at the sensing nanostructures<sup>1</sup>.

In the second part we present the integration of droplet-based microfluidics on silicon nanowire field effect transistors (SiNW FETs) and the successful label-free detection of water-on-oil droplets uniquely based on the ionic environment of the passing liquid phases. Based on the sensitivity of SiNW FETs on the pH value in liquid surroundings<sup>2</sup>, we show the detection of aqueous droplets with various physiological pH values, ranging from 4 to 8. Finally, we demonstrate the capability of the developed hybrid device for *lab-on-a-chip* applications by monitoring the pH change of passing droplets introduced by the oxidation of glucose to gluconic acid, probed into the droplet-containing phase (See figure 1, panel B)<sup>3</sup>.



**Figure 1:** A) Schematic illustration of the nano capacitor sensing device. The analyte solution is guided between the gold nanowire electrode pair thereby altering the impedance of the sensing structure. B) Working principle of label-free droplet detection using SiNW FETs. The droplets are detected purely by their ionic environment. Furthermore, droplet stem solution is probed with glucose and the enzyme glucose oxidase, resulting in the oxidation of glucose to gluconic acid thereby altering the pH value of propagating droplets.

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#### 3D Ordered Porous Polydopamine as HCHO and CO<sub>2</sub> Gas Sensor

#### Wenbo Sheng, Rainer Jordan\*

Professur für Makromolekulare Chemie, Department Chemie, Technische Universität Dresden, Mommsenstrasse 4, 01069 Dresden, Germany

To meet the increasing requirements for gaseous chemical detection, various new sensing materials have been designed and developed to improve the sensing performance of chemical sensors.<sup>[1,2]</sup> Among the various synthesis strategies, the bio-inspired process plays an important role in the new material development. Inspired from this interesting phenomenon, in 2007, Lee et al., reported that dopamine with both catechol and amine groups, was an ideal building block to form an adhesive polydopamine film onto various surfaces like polymers and metals.<sup>[3]</sup> More importantly, as for advanced material design by using this bio-inspired method, kinds of nanostructures with interesting shapes like hollow nanocapsules have been successfully prepared.<sup>[4-6]</sup> In this work, we report a bio-inspired synthesis of 3D porous polydopamine material with desired flexibility and their future application for HCHO and  $CO_2$  gas sensing. The porous structure provides higher surface area to volume ratio and which contributes in the gas diffusion process and results in the improvement of the gas sensing properties. This work is highly desirable to develop a more facile approach under mild reaction conditions and use a greener method to prepare sensor and improve its detection sensitivity.

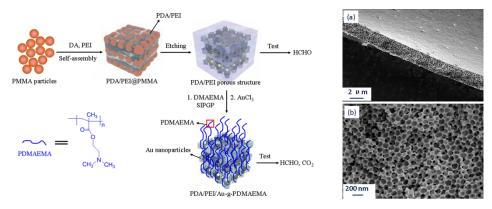


Figure 1. (Left) Schematic illustration of the synthesis of PDA/PEI and PDA/PEI-g-PDMAEMA porous sensor; (Right) SEM images of PDA/PEI porous structure: (a) section of the sample, (b) enlarged portion.

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#### Donor-acceptor-donor molecules for on-surface polymerization

Dmitry Skidin<sup>1</sup>, Frank Eisenhut<sup>1</sup>, Justus Krüger<sup>1</sup>, Tim Erdmann<sup>2,3</sup>, Anton Kiriy<sup>2,3</sup>,

Brigitte Voit<sup>2,3</sup>, Gianaurelio Cuniberti<sup>1,2</sup>, and Francesca Moresco<sup>1,2</sup>

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

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

<sup>3</sup>Leibniz-Institut für Polymerforschung Dresden e.V., 01069 Dresden, Germany

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

One of the main tasks of the modern molecular electronics is the formation of supramolecular structures that could serve as functional units for the circuitry at nanoscale. In this regard molecular wires with high conductivity are of essential importance. Apart from conductivity, other crucial properties are finite band gap and flexibility. However, for the most of the well-studied molecular wires systems some of these characteristics had to be sacrificed for the benefit of the others. Therefore, it was suggested to use the molecules with alternating donor and acceptor units as monomers for flexible conductive wires with non-zero band gap<sup>1</sup>.

We employ conjugated diketopyrrolopyrrole-based molecules of the donor-acceptor-donor type to grow organic polymers on the surface. After the deposition of individual brominated monomers on Au(111) surface the sample is annealed in order to promote activation and diffusion of molecules leading to polymerization in a reaction known as Ullmann coupling. After molecular wires are formed and stabilized on the surface, their structural and electronic properties can be studied using low-temperature scanning tunneling microscopy and spectroscopy.

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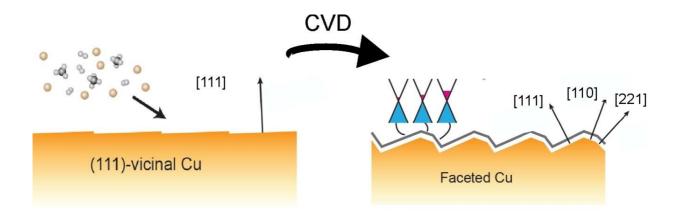
# Nanofaceting as a stamp for periodic graphene charge carrier modulations

<u>M. Vondráček<sup>1</sup></u>, D. Kalita<sup>2</sup>, M. Kučera<sup>1</sup>, L. Fekete<sup>1</sup>, J. Kopeček<sup>1</sup>, J. Lančok<sup>1</sup>, J. Coraux<sup>2</sup>, V. Bouchiat<sup>2</sup> and J. Honolka<sup>1</sup>

<sup>1</sup>Institute of Physics of the Czech Academy of Sciences, CZ-182 21 Prague 8, Czech Republic <sup>2</sup>Département Nanosciences, CNRS, Institut Néel, F-38042 Grenoble, France

Corresponding author: vondrac@fzu.cz

Reduced symmetry conditions on high-index vicinal copper surfaces are exploited to efficiently imprint well-defined structural and electronic modulations in continuous graphene sheets. The combination of conventional microscopy with wave vector resolved photoemission electron microscopy (*k*-PEEM) allows to locally distinguish different levels of interaction of graphene with three coexisting copper facets (111), (110), and (221), which lead to alternating doping levels at the nanoscale. Ordering is driven by surface energy minimization, inducing anisotropic copper and carbon mass-transfers during high temperature chemical vapor deposition. The results have been recently published [1].



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[1] Vondráček et al., Scientific Reports 6, 23663 (2016). http://dx.doi.org/10.1038/srep23663

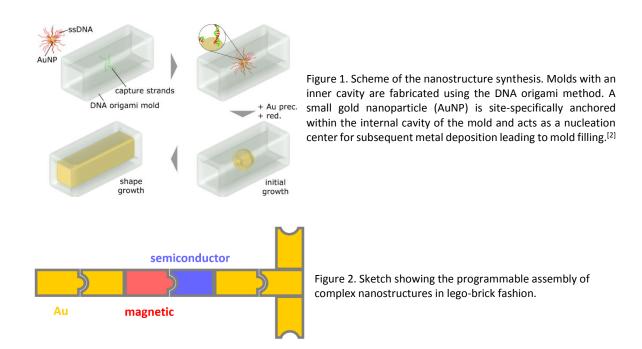
# Nano-electronic components built from DNA templates

Jingjing Ye, Seham Helmi, Ralf Seidel

Institute of Experimental Physics I, Universität Leipzig, Linnéstr. 5, 04103 Leipzig, Germany

Email: ralf.seidel@physik.uni-leipzig.de

On the nanoscale fundamental properties and potential applications are greatly influenced by the size and shape of the material. "DNA Origami" takes advantage of base complementarity of individual short oligonucleotides, to fold a long "scaffold strand" into almost any continuous 2D or 3D shape.<sup>[1]</sup> We recently introduced a new concept of DNA mold-based particle synthesis that allows the synthesis of inorganic nanoparticles with programmable shape. We demonstrated the concept by fabricating a 40 nm rod-like gold nanostructure with a quadratic cross-section (see Figure 1).<sup>[2]</sup> We also expand the capabilities of the mold-based particle synthesis to demonstrate the synthesis of uniform gold nanowires with controllable dimensions. Using magnetic beads as solid-support to assemble 'supermold' also provides a unique and flexible way to fabricate complex inorganic nanostructures in a lego-brick like fashion from uniform building blocks (mold monomers). Different materials can grow inside each mold monomer to achieve new material combination (see Figure 2). In addition, double stranded DNA layer with high spin-selectivity can be used as efficient spin filter for spintronic applications.



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#### Site-specific attachment of a semiconducting polythiophene-derivate to DNA origami structures

J. Zessin<sup>1,2</sup>, F. Fischer<sup>1,2</sup>, A. Heerwig<sup>2,3</sup>, A. Kick<sup>3</sup>, M. Stamm<sup>1</sup>, A. Kiriy<sup>1</sup>, M. Mertig<sup>1,3</sup>

#### zessin@ipfdd.de

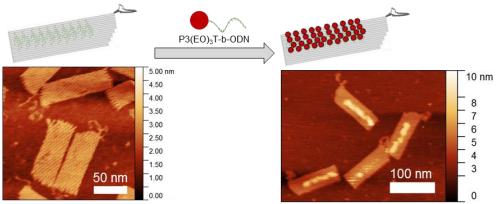
<sup>1</sup>Leibniz-Institut für Polymerforschung Dresden e.V., 01069 Dresden, Germany

<sup>2</sup>Phys. Chemie, Mess- und Sensortechnik, Technische Universität Dresden, 01062 Dresden, Germany

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

DNA-based structures that rely on the distinctive recognition properties of DNA have recently shown their potential to act as molecular "breadboards" for the arrangement of functional heteroelements. DNA origami [1] is one of the most promising approach due to its structural variety and stability. Such functional heteroelements can be conjugated polymers (CPs). These organic (semi)-conductors are characterized by appealing optical and electronic properties. Compared to inorganic particles, they furthermore captivate due to their light-weight and flexibility. They are applicable in diverse electronic and optoelectronic devices. To date, only few approaches have appeared to attach CPs on DNA origami structures [2, 3]. Here, we present a new way to attach CPs onto a DNA origami structure. In contrast to the previous reports, we used a controlled polymerization, the so called Kumada catalyst-transfer polycondensation, which leads to narrow distributed polymers with adjustable molecular weights and start/end groups [4].

First, we prepared the water-soluble, semiconducting polythiophene,  $P3(EO)_3T$  having oligoethylene glycol side chains. An amine-starting group was introduced via a functionalized catalyst that gives access to facile click chemistry. Accordingly, the  $P3(EO)_3T$  was bound to an end-modified, synthetic oligodeoxynucleotide (ODN) yielding to the block copolymer  $P3(EO)_3T$ -b-ODN. First, the hybridization performance of the block copolymer was studied in a microfluidic system using surface plasmon resonance spectroscopy for the detection of surface-bonding events. We observed a comparable hybridization performance of the block copolymer to the bare ODN that proofs the DNA-binding capability of the block copolymer. Next, the attachment behavior was studied on a rectangular 2D DNA origami, the so called pad. The pad bears single-stranded overhangs in different patterns and sequences (15A and specific sequence). These hybrid structures were investigated by liquid, high-resolution AFM. In both cases we achieved the site-specific attachment yielding to the hybrid P3(EO)\_3T@pad.



**Figure 1**. Schematic presentation and high-resolution AFM images of the site-specific attachment of  $P3(EO)_3T$ -b-ODN to the DNA origami pad yielding to the hybrid structure  $P3(EO)_3T$ @pad.

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#### Stimulus-responsive micro-supercapacitors with ultrahigh energy

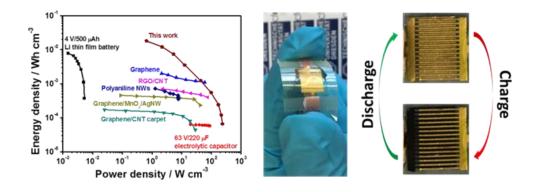
#### density and reversible electrochromic window

Panpan Zhang, Prof. Dr. Xinliang Feng

Center for Advancing Electronics Dresden (cfaed) & Department of Chemistry and Food Chemistry, Technische Universität Dresden, 01062 Dresden, Germany.

#### Abstract:

Stimuli-responsive energy storage devices have become an emerging field in recent years. However, the introduction of stimuli usually results into sacrificed device performance that has thus far restricted their potential for practical applications. Here we report a strategy to realize stimulus-responsive and high energy density for flexible micro-supercapacitors (MSCs) by using viologen and graphene/ $V_2O_5$  hybrid nanopaper as stimulus-responsive component and active electrode, respectively. The 1D pseudocapacitive  $V_2O_5$  nanoribbons, 2D conductive exfoliated graphene nanosheets and electrochromic viologen, together contribute to such stimulus-responsive high-energy MSCs. Our results suggest that the development of high performance stimuli-responsive energy storage devices with enhanced human-device interaction experience becomes possible.



#### NanoNet International Workshop 2016, Prague

Conference Dinner – Thursday, 7.30 p.m. - Menu

Pálffy Palác

Pálffy Palác restaurant, Valdštejnská 14, 118 00 Praha 1 – Malá Strana T: +420 257 530 522 M: +420 602 711 230 E: <u>palffy@palffy.cz</u> W: <u>www.palffy.cz</u>

#### Starter

S1	Pumpkin soup with roasted pumpkin seeds or
S2	Goat cheese gratinated with honey served with baked apples and shredded lettuce
Main Course	
M1	Lamb shoulder braised 9 hours in red wine and rosemary served with Parmesan spinach leaves and sautéed potatoes or
M2	Butter fish fillet with piquant parsnips served with sautéed spinach and shallots vinaigrette or
М3	Cous Cous with mixture of vegetables
Dessert	
D1	Lavender Crème brûlée or
D2	2 pcs of Profiterolls filled with icecream and topped with hot chocolate



Directions: 1) walk by about 35 min. 2) take tram no. 12 (dir. Palmovka) or no. 20 (dir. Nadrazi Podbada) until 'Malostranske Namesti' (5 stops)

#### NanoNet International Workshop 2016, Prague

#### Participants

#### Updated: 25.08.2016 (PZ)

Name	First Name	Gender	Title	Institution
Ahmed	Omair	Mr.		HZDR
Arasu	Narendra	Mr.		FZU Prague
Arora	Himani	Ms.		HZDR
Awan	Wajid	Mr.		HZDR
Baek	Eunhye	Ms.		TU Dresden
Baraban	Larysa	Mrs.	Dr.	TU Dresden
Bayrak	Türkan	Ms.	51.	HZDR
Bogani	Lapo	Mr.	Dr.	U Oxford
Bouchiat	Vincent	Mr.	Dr.	CNRS Grenoble
	Taras	Mr.	DI.	
Chutora			Dest De	FZU Prague
Cuniberti	Giovanni	Mr.	Prof. Dr.	TU Dresden
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Fikáček	Jan	Mr.	Dr.	FZU Prague
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Gemming	Sibylle	Mrs.	Prof. Dr.	HZDR
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Günther	Florian	Mr.		HZDR
Honolka	Jan	Mr.	Dr.	FZU Prague
Jariwala	Deep	Mr.	Dr.	Caltech
Joshi	Vinayakrishna	Mr.	5	HZDR
Kalbac	Martin	Mr.	Dr.	UFCH-CAS Prague
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Kelling	Jeffrey	Mr.	DI.	HZDR
<b>v</b>		Mr.		
Khan	Bilal			HZDR
Kilibarda	Filip	Mr.		HZDR
Kiriy	Anton	Mr.	Dr.	IPF Dresden
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Kratochvilova	Irena	Mrs.	Asc.Prof. Dr.	FZU Prague
Krstić	Vojislav	Mr.	Prof. Dr.	U Erlangen
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Pacáková	Barbara	Ms.		FZU Prague
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Vondráček	Martin	Mr.		FZU Prague
Ye	Jingjing	Ms.		U Leipzig
Zahn	Peter	Mr.	PD Dr.	HZDR
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Zhang	•			
Zhuravel	Roman	Mr.		U Jerusalem



