

International Helmholtz Research School
for Nanoelectronic Networks



IHRS NANONET Annual Workshop 2014

29/30 September 2014, Berghotel Bastei
Germany



Venue and organization

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Agenda

updated 18.09.2014 (PZ)

Monday, 29 September 2014

Start	Who	Duration (min)	What	Notes
~11:00			Transfer from Pirna/ Hiking from Rathen	
12:30			Arrival/Lunch Snacks	Chair: A. Erbe
14:00	Artur Erbe	10	Welcome address	
14:10	Yordan Georgiev	40+10	Si nanowires	
15:00		20	Break	Chair: S. Gemming
15:20	Andrey Turchanin	40+10	2d nano membranes	
16:10	Anna Delin	40+10	Nanoscale transport	
17:15		90	Posters with drinks / voting	
18:30		30	Finish voting / Count votes	
19:00			Dinner including poster prize ceremony	
~20:30		60	Steering committee meeting	

Tuesday, 30 September 2014

7:00			Breakfast	Check-out 10:30 Chair: M. Helm
9:00	Artur Erbe	25+5	NanoNet overview	
9:30	Stefan Facsko	25+5	Nanowire epitaxy	
10:00	Walter Weber	25+5	Si nanowires	
10:30		20	Break	Chair: S. Facsko
10:50	Sibylle Gemming	25+5	Transport theory	
11:20	Teresa Gonzalez	40+10	STM break junctions	
12:30			Lunch	
~14:00			Departure	

Talk abstracts

M. T. González

Electrical properties for circuits based in single organic molecules

Andrey Turchanin

A molecular way to 2D carbon materials for electronic applications

Anna Delin

Nanoscale transport

Artur Erbe

NanoNet goals and vision

Stefan Facsko

Spontaneous pattern formation on ion irradiated surfaces

Walter M. Weber

Group IV - Nanowire Electronics

Sibylle Gemming

Calculating transport through nanostructures

Yordan M. Georgiev

Top-down fabrication and some applications of Si and Ge nanowires

Electrical properties for circuits based in single organic molecules

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The realization and study of molecular junctions formed by a few (down to one) molecules bonded between two metallic electrodes opens the possibility of directly investigating electrical properties of compounds at the ultimate level of a single molecule. Apart from the determination of their electrical conductance, it is important to understand which factors play a role in the formation and breakage of the molecular junctions, and how stable we can expect them to be.

In this presentation, I will summarize some of the most relevant achievements in the field in the last 10 year. I will describe the most successful approaches to form and study molecular junctions, as well as the most inspiring organic compounds synthesized as possible components of nano-scale electronic circuits. I will then present our studies on the molecular junctions formed by simple organic molecules. We use a STM (scanning tunneling microscope) to create and characterized single-molecule junctions using different techniques. We use the versatile break-junction technique to explore the compounds terminated by thiol-, amine-, and SMe-groups [1], while we have developed an specific approach for the 'targeted wiring' of molecules terminating in C₆₀ [2]. We also performed simultaneous conductance and thermopower measurements on molecular junctions [3], showing the potential of inter-molecular interactions manipulation for increasing the thermopower.

References

- [1] M. T. González et al. *J. Am. Chem. Soc.* **135**, 5420–5426 (2013); M. T. González et al., *J. Phys. Chem. C* (2014) DOI: 10.1021/jp506078a.
- [2] E. Leary et al. *Nano Lett.* **11**, 2236 (2011); K. Guillemot et al. *Small* **9**, 3812 – 3822 (2013).
- [3] C. Evangeli et al., *Nano Lett.* **13**, 2141–2145 (2013).

A molecular way to 2D carbon materials for electronic applications

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In this talk it will be demonstrated how monolayers of aromatic molecules are employed to engineer novel free-standing 2D carbon materials. By electron or photon irradiation, aromatic monolayers are converted into dielectric carbon nanomembranes (CNMs) with a thickness of one molecule, which can be tuned from ~0.5 to 3 nm. CNMs possess high mechanical stability and similar to graphene or other atomically thin 2D materials (e.g., hBN, MoS₂) can be separated from their original substrates and transferred onto various other substrates, fabricated as suspended sheets or stacked into multilayer films with precise control over their thickness. By annealing CNMs are converted into graphene. This approach enables both scalable productions of graphene and direct writing of CNM or graphene micro and nanostructures employing e-beam or extreme UV lithography. Layer-by-layer assembly of vertical CNM/graphene heterostructures opens many doors to the engineering of novel materials with tunable electronic, optical and chemical properties. Their characterization by complementary spectroscopy, microscopy, electric and magnetoelectric transport measurements as well as implementation in novel field-effect devices will be presented.

References

- [1] M. Woszczyna et al.: All-carbon vertical van der Waals heterostructures: Non-destructive functionalization of graphene for electronic applications. *Adv. Mater.* 26 (2014) 4831-4837
- [2] D. G. Matei et al.: Functional single-layer graphene sheets from aromatic monolayers. *Adv. Mater.* 25 (2013) 4146-4151
- [3] P. Angelova et al.: A universal scheme to convert aromatic molecular monolayers into functional carbon nanomembranes. *ACS Nano* 7 (2013) 6489-6421
- [4] A. Turchanin and A. Götzhäuser: Carbon nanomembranes from self-assembled monolayers: Functional surfaces without bulk. *Prog. Surf. Sci.* 87 (2012) 108-162

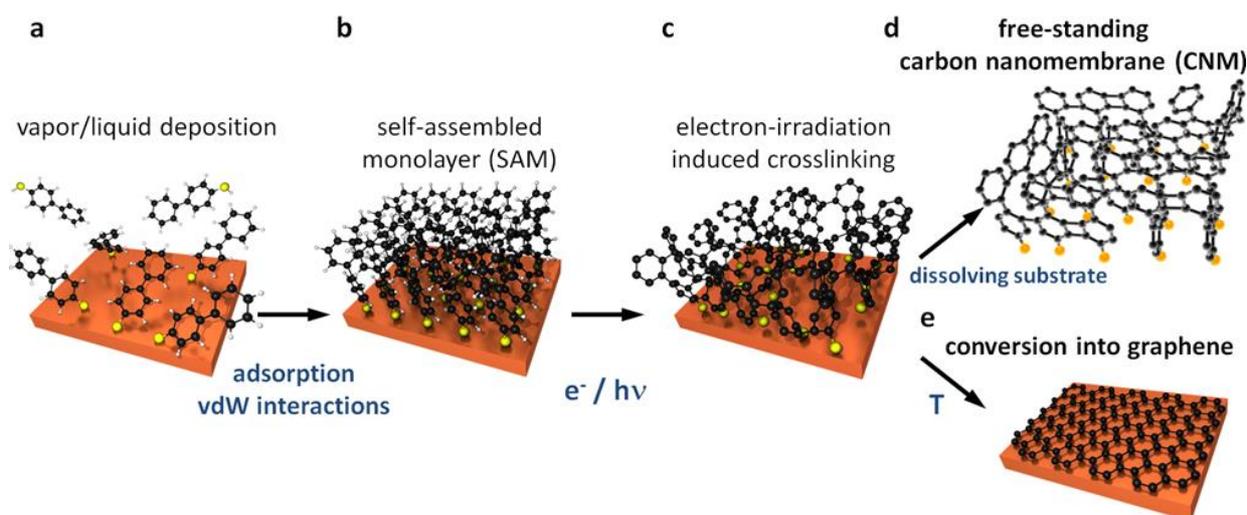


Fig. 1: Schematic of the fabrication route to carbon nanomembranes (CNMs) and graphene from aromatic self-assembled monolayers (SAMs): a, Deposition of molecules on a substrate; here, vapor deposition of biphenyl-thiols (BPT). b, Formation of a SAM. c, Electron/photon-irradiation-induced crosslinking of the BPT SAM into a carbon nanomembrane (CNM). d, Formation of a free-standing CNM via dissolving the substrate. e, Conversion of the CNM into graphene via annealing.

Nanoscale transport

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Confinement or a small length scale in one or more dimensions can have profound consequences for transport phenomena. In this talk, which I intend to be tutorial in character, I will point out and discuss the physics of some fascinating transport phenomena in such structures, in particular quantized conductance, spin transport in molecules, as well as spin thermoelectric phenomena.

NanoNet goals and vision

Artur Erbe

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The International Helmholtz Research School (IHRS) NanoNet school aims at the creation of nanoelectronic circuits, which are based on the interaction of various building blocks linked together on the nanometer scale. This goal can only be achieved if a team of experts in the fields of physics, chemistry, and electrical engineering combine their efforts in defining new structures and new methods of interlinking these structures. In this presentation, I will give an overview on the single building blocks, their synthesis and function, as well as on the development of the interlinking schemes. The figure below shows highlights of systems, which have been built and characterized in the collaborations in the school. Special emphasis will be given to the electrical functionalities of the nanoscale building blocks, which eventually will allow their use in nanoelectronic circuits. Examples are single molecular switches (**a**), self-organized and self-oriented DNA origami structures (**b**), and wires, which switch their conductance by changes in their structure (**c**). In addition to conventional electrical characterization we also show novel characterization methods, which are essential for the detailed understanding of the behavior of the nanostructures. Based on this information, theoretical models for the single nanostructures and their connections to conducting leads are built which, in turn, make the development of larger circuits possible. These are the essential parts for the development of nanoelectronic networks.

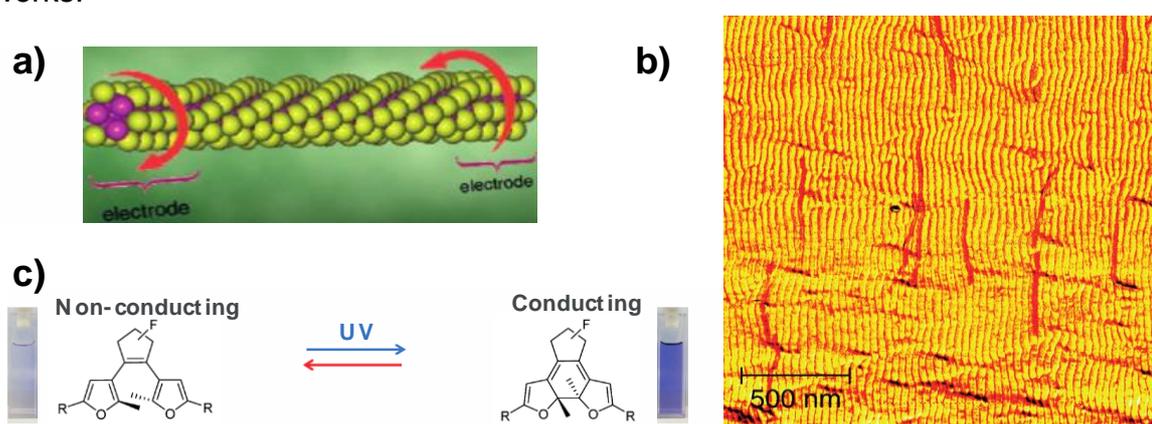


Figure 1 **a)** MoS_x wire changing its conductance value upon torsion **b)** DNA origami nanorods oriented on self-organized silicon surface ripples¹. **c)** Photosensitive single-molecule switch.

Reference

1. B. Teshome, S. Facsko, and A. Keller, *Topography-controlled alignment of DNA origami nanotubes on nanopatterned surfaces*, *Nanoscale* **6**, 1790 (2014).

Spontaneous pattern formation on ion irradiated surfaces

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In molecular beam epitaxy (MBE) the continuous deposition of atoms on a surface can lead to growth of self-organized 3D nanostructures. One of the possible surface instability, which is responsible for this kind of growth is caused by the Ehrlich-Schwoebel (ES) barrier, i.e. an additional diffusion barrier for ad-atoms crossing terrace steps [1]. Therefore the deposited atoms are trapped on terraces and nucleate to form new terraces. This mechanism leads to the growth of pyramidal mounds with facets corresponding to energetically favored crystal planes. An analogous mechanism is also observed on ion irradiated surfaces. Ion sputtering leads to surface erosion by sputtering and at room temperature semiconductor surfaces become amorphous. At these conditions periodic patterns are observed which are oriented perpendicular or parallel to the ion beam direction or are isotropic dot or hole patterns for normal incidence of the ion beam [2].

However, at temperatures above the recrystallization temperature of the material, bulk defects are dynamically annealed and amorphization is prevented. Now, ion sputtering is creating vacancies on the crystalline surface and the morphology is determined primarily by vacancy kinetics. The diffusion of vacancies is also biased by the ES barrier in analogy to the diffusion of ad-atoms. Consequently, the 3D growth turns into a 3D erosion. The resulting spontaneous surface patterns consist of inverse pyramidal structures which are growing into the material [3]. The symmetry of these self-organized patterns is given by the crystal symmetry of the surface. Hence, checkerboard patterns appear on the Ge (001) surface, oriented in the $\langle 100 \rangle$ directions. On the other hand, on the Ge (111) surface facets with a three-fold symmetry evolve. For high ion fluences the patterns also exhibit facets, which correspond to low index crystal planes.

For the description of the pattern formation and evolution in reverse epitaxy a continuum equation can be used, which combines the effects of ion irradiation and effective diffusion currents due to the ES barrier on the crystalline surface. By including also a conserved Kardar-Parisi-Zhang term a remarkable qualitative agreement to the experiments is achieved [3].

References

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[2] A. Keller, S. Facsko, Materials **3**, 4811 (2010).

[3] X. Ou, A. Keller, M. Helm, J. Fassbender, S. Facsko, Phys. Rev. Lett. **111**, 016101 (2013).

Group IV - Nanowire Electronics

Walter M. Weber^{1,2}, André Heinzig^{2,3}, Matthias Grube^{1,2}, Jens Trommer^{1,2}, Sebastian Pregl^{1,2}, Tim Baldauf^{2,3}, Jürgen Beister¹, Dae-Young Jeon^{2,3}, So-Jeong Park^{2,3}, Andreas Krause^{1,2}, and Thomas Mikolajick^{1,2,3}

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Silicon and Germanium nanowire transistors with diameters well below ten nanometers hold the promise of combining one-dimensional transport phenomena with the advantageous CMOS fabrication schemes. In this talk we will review the advances, opportunities and limitations of both bottom-up assembled and top-down processed Silicon and Germanium nanowire transistors. Special emphasis will be given in the suitability of these devices to solve system related necessities. Following an overview we will focus on the one-dimensional contact properties of metals to semiconductors [1,2]. The sharp interfaces and efficient electrostatic control are exploited to enable the realization of reconfigurable field effect transistors (RFETs) [3,4]. These functionality enhanced four-terminal devices deliver n- and p-FET switching characteristics from the same device as selected simply by an electric signal and without the need for doping. Future computing circuits can make use of this reconfiguration method and low operating and standby power concept to perform multiple logic operations with the same hardware. [5] We will further show how low dimensionality can lead to the enhancement of output characteristics [6]. The meso-scopic effects are further employed in printed parallel nanowire arrays to yield high current transistors [7].

References:

- [1] W. M. Weber et al. "Silicon-nanowire transistors with intruded nickel-silicide contacts" *Nano Letters* **6**, pp. 2660-2666 (2006)
- [2] D. Martin, A. Heinzig, M. Grube, T. Mikolajick, L. Geelhaar, H. Riechert and W. M. Weber "Direct probing of Schottky barriers in Si nanowire Schottky barrier FETs" *Phys. Rev. Lett.* **107**, 216807 (2011)
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- [5] J. Trommer et al. "Elementary Aspects for Circuit Implementation of Reconfigurable Nanowire Transistors" *Electron Device Letters* (IEEE) **35**, p. 141 (2014)
- [6] W. M. Weber et al. "Reconfigurable nanowire electronics – A review" *Solid State Electronics* DOI: 10.1016/j.sse.2014.06.010 (2014)
- [7] S. Pregl et al. "Parallel arrays of Schottky barrier nanowire field effect transistors: nanoscopic effects for macroscopic current output" *Nano Research* **6**, pp. 381-388 (2013)

Calculating transport through nanostructures

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Spatial confinement effects induce fascinating new phenomena in nanostructured media, which are based on structure- and surface-controlled modifications of the bulk material properties. A thorough understanding of the resulting properties and an assessment of the application potential ideally relies on a combination of experimental and modelling techniques, which cover the whole range of nanostructure creation, characterization and applicative integration into larger functional elements. Thus, we apply self-organized patterning by ion-beam-induced surface modifications and top-down electron lithographic techniques to generate nano-scale functional elements and combine it with nanometrology methods on specific structural, mechanical, optical and transport phenomena and with scale-adapted as well as multi-scale modeling.

Transport properties on the small scale, for instance, have traditionally been addressed by a classical master equation approach for the motion of the different charge carrier species, which is based on rate theory. The rather large quantity of parameters, which enter such an approach, can more or less easily be adjusted to the dimensional characteristics, local potential changes at interfaces, and the electronic settings of the system as well as to temperature effects. On the other hand, a microscopically more detailed and mostly parameter-free picture is obtained from a quantum-mechanical treatment on the basis of the density-functional theory. An extension by a Green's function formalism allows treating the response to an applied external field and thus the determination and analysis of electronic transport through contacted nanostructures within the limits of a perturbative ansatz. Systems with more complicated electronic response to external triggers may even exhibit many-body effects, which require an explicit treatment by multi-reference calculations. We have combined these approaches to study electron transport in several material systems with different degrees of structural and electronic complexity.

Top-down fabrication and some applications of Si and Ge nanowires

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Semiconductor nanowires (NWs) have extensively been studied for the last two decades due to their attractive electronic, photonic, thermal, electrochemical and mechanical properties and large surface area to volume ratios. They can be produced in good quality and reasonable quantities from 'bottom-up' synthetic methods, however, their post positioning, alignment, and integration remains a challenge. These issues are easily overcome by producing arrays of nanowires from 'top-down' methodologies, e.g. electron beam lithography (EBL) and reactive ion etching (RIE). The top-down approach also allows better control over nanowire length, width, thickness, number, and orientation along different crystallographic axes.

In this talk results on top-down fabrication of arrays of complex Si NW devices having different widths (10, 20, 30, and 50 nm), lengths (0.5, 1, and 10 μm), and numbers (1, 3, and 20) of nanowires will be presented [1, 2]. The fabrication is based mainly on high-resolution EBL and pattern transfer by RIE. The key factors for achieving small widths and smooth surfaces of the nanowires will briefly be discussed. The excellent electrical parameters of fabricated devices as well as their superb performance as chemo/biosensors will be demonstrated. To the best of our knowledge, they are the smallest top-down fabricated Si NW sensors reported to date having the highest sensitivity towards the protein streptavidin.

In addition, an advanced technology for fabrication of sub-5 nm suspended Si NWs will be described in general.

Finally, the motivation for working with germanium as an alternative to Si will be discussed, together with the challenges arising during its processing. Options for high-resolution patterning of Ge will be proposed and Ge NWs having widths of 20 nm and below will be demonstrated, which are the smallest top-down fabricated Ge NWs reported so far. Two different applications of these NWs will briefly be presented: (i) development of alternative methods for non-defective doping of nanostructures and (ii) fabrication of Ge junctionless nanowire transistors, the first Ge transistors of this novel type demonstrated to date [2, 3].

[1] Y. M. Georgiev et al., Fully CMOS-compatible top-down fabrication of sub-50 nm silicon nanowire sensing devices, *Microelectron. Eng.* **118**, 47-53 (2014).

[2] Y. M. Georgiev et al., *Silicon and Germanium Junctionless Nanowire Transistors for Sensing and Digital Electronics Applications*, in "Functional Nanomaterials and Devices for Electronics, Sensors and Energy Harvesting", A. Nazarov et al. (eds.), Springer International Publishing AG, Cham, Switzerland, in press.

[3] R. Yu, Y. M. Georgiev et al., Junctionless Nanowire Transistor fabricated with high mobility Ge channel, *Phys. Status Solidi Rapid Research Letters (RRL)* **8**, No. 1, 65–68 (2014).

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Your Notes

Poster abstracts

Yuriy Aleksandrov

Evolution of the perpendicular magnetic anisotropy on CoFeB/MgO based multilayer by annealing temperature

Eunhye Baek

Optoelectronic Switching of Nanowire-based Hybrid Organic/Oxide/Semiconductor Field-Effect Transistors

Dipjyoti Deb

Top-down fabrication and characterization of reconfigurable silicon nanowire field effect transistor

Florian Günther

Electronic Structure Calculations on donor-acceptor polymers

Mimi Hetti

Synthesis and Characterization of Functionalized Magnetic Nanoparticles

Banu Iyisan

Multifunctional polymersomes with photoactive moieties and their non-covalent attachment onto surfaces

Jeffrey Kelling

Elastic Properties of Nickel Carbides

Lokamani

Electronic structure of photosensitive molecular switches: A first-principle investigation

Jonas F. Nawroth

Surface Patterning and Positioning of DNA Origami on the Nanoscale

Gözde Öktem

Synthesis of well-defined bis-functionalized semiconducting oligomers for single molecule nanoelectronics

Torsten Sandler

Electrical characterization of in-situ switched diarylethene single molecule junctions

Bezuayehu Teshome

Heterogeneous nanoparticle assemblies on DNA Origami

Evolution of the perpendicular magnetic anisotropy on CoFeB/MgO based multilayer by annealing temperature

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Magnetic tunnel junctions with perpendicular magnetic anisotropy (PMA) are good candidates for next generation spin-transfer torque magnetic random access memory (STT-MRAM) [1]. PMA STT devices offer a better trade-off between maintaining sufficient thermal stability, while allowing for comparatively lower switching currents than in-plane magnetized films. In addition, the recently reported appearance of PMA in MgO/CoFeB/Ta structures enables the design of devices with high quality MgO barriers and consequently high tunneling magnetoresistance (TMR) ratios.

We focus on studying the change in magnetic anisotropy versus annealing temperature (T_A) for MgO 2\Co₄₀Fe₄₀B₂₀ 1\Ta 5\Ru 5 (thickness in nm) multilayers through analyzing the angular dependence of ferromagnetic resonance (FMR). The samples were grown by RF and DC sputtering using a TIMARIS cluster deposition tool [2], and annealed in N₂ environment for 30 minutes at temperatures between 150°C and 250°C, in steps of 50°C. FMR measurements are performed at room temperature using a microwave cavity [3].

In the as-deposited state, the CoFeB is amorphous while the MgO is weakly textured (001). Upon annealing, crystallization proceeds from the MgO interface into the CoFeB layer resulting in an ordered (001) bilayer with a small lattice mismatch [4]. The appearance of PMA in such systems has been attributed to the hybridization of Fe and O orbitals [5]. We find that, while for all for the considered T_A the magnetization easy axis remains perpendicular to the plane of the layers, the effective perpendicular anisotropy increases with increasing T_A , as the crystalline structure becomes more ordered. However, the angular dependence of the FMR spectra cannot be accounted for assuming solely a uniaxial PMA and additional anisotropy contributions have to be taken into account. FMR measurements also show a secondary peak, which has a typical narrow paramagnetic-like behavior and may arise from paramagnetic defects diffusing into the MgO layer. This signal initially has a cubic symmetry and changes to tetragonal-like behavior with increasing T_A .

References

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Optoelectronic Switching of Nanowire-based Hybrid Organic/Oxide/Semiconductor Field-Effect Transistors

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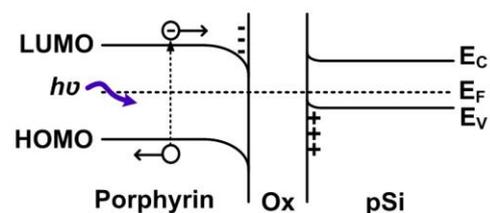
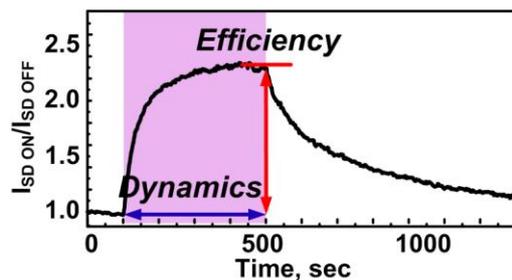
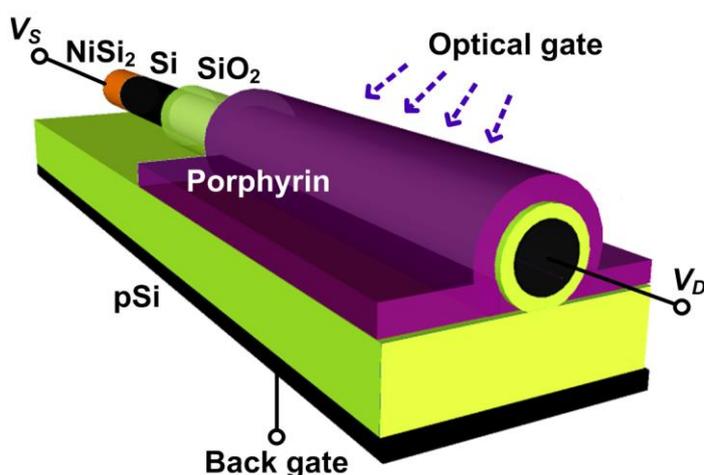
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We present a novel photosensitive hybrid nanowire-based field-effect transistor (FET) which consists of the multiple-shell of organic porphyrin film/oxide/silicon nanowire. Due to the oxide shell around the nanowires, photo-switching of the current in the hybrid nano-devices is guided by the field effect, which is induced by charge redistribution within the organic film. This principle is an alternative to a photo-induced electron injection, valid for devices relying on direct junctions between organic molecules and metals or semiconductors. We investigate the switching dynamics of the hybrid nano-devices upon violet light illumination and find a strong dependence on the thickness of the porphyrin film wrapping the nanowires. Furthermore, the thickness of the organic films is found to be a crucial parameter also for the switching efficiency of the nanowire FET, represented as the ratio of currents under light illumination (ON) and in dark conditions (OFF). We suggest a simple model of porphyrin film charging to explain the optoelectronic behavior of nanowire FETs mediated by organic film/oxide/semiconductor junctions.



Top-down fabrication and characterization of reconfigurable silicon nanowire field effect transistor

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The following work illustrates top-down fabrication and characterization of reconfigurable, undoped silicon nanowire field effect transistors with Schottky junctions. The nanowires are fabricated on SOI substrates by electron beam lithography followed by reactive ion etching. The mixed gas etch recipe is optimised to etch silicon nanowires with 50 nm width, 200 nm height and 1.5 μm to 2 μm length as illustrated in fig 1.1. Two nickel-silicide Schottky junctions are formed by nickel sputtering and annealing from source and drain region creating silicide-silicon-silicide contacts as illustrated in fig 1.2. Diffusion of Ni-Si is controlled by radial crystal orientation of the nanowire and annealing temperature [1].

The Schottky junctions are electrostatically controlled by a top gate. The nanowire is expected to demonstrate bipolar $I_D - V_G$ characteristics for the positive and negative half of the voltage sweep [2].

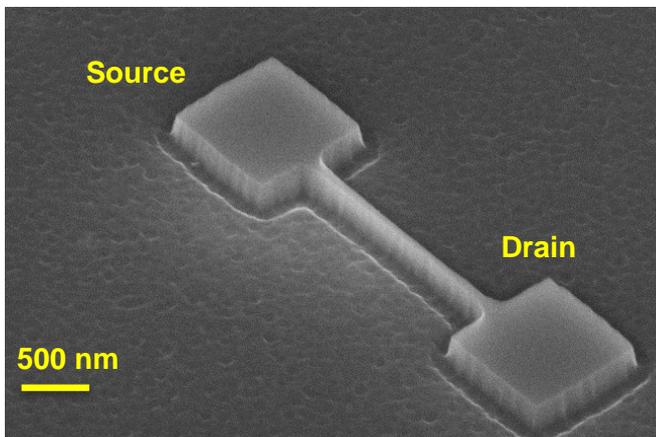


Fig 1.1: Silicon Nanowire (height = 200 nm, width = 50 nm, length = 1.2 μm) on silicon substrate etched with SF_6/O_2 mixed gas reactive ion etching.

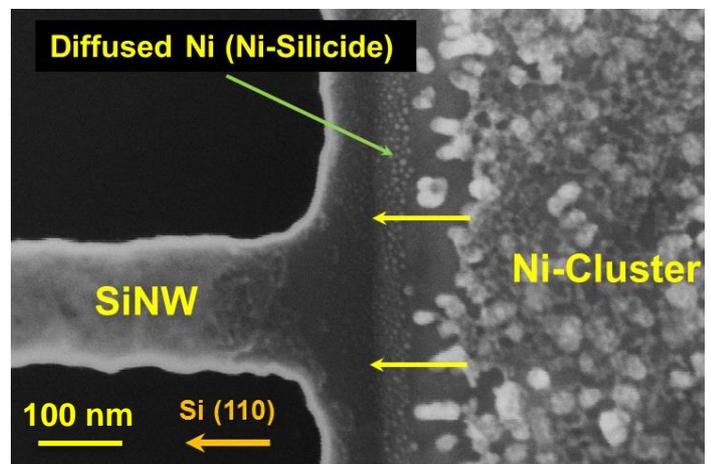


Fig 1.2: Diffusion of sputtered nickel in silicon substrate. After annealing at 450° C for 50 sec in forming gas atm.

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Electronic Structure Calculations on donor-acceptor polymers

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

In order to analyze the influence of the molecular structure on these properties, we investigate DA polymers using first-principles methods as density functional theory (DFT). In particular, density functional based tight binding (DFTB) is used to study large systems.

Starting from isolated monomers being the building blocks of the DA polymers the total energy, the atomic charges, the difference between highest occupied and lowest unoccupied molecular orbitals, and the reorganization energies are calculated.

Furthermore, oligomers up to a length of 100 conjugated units as well as infinite long polymers are considered. Finally, the morphological properties are investigated by studying systems of several polymer chains with different crossing angles and relative shifts.

Synthesis and Characterization of Functionalized Magnetic Nanoparticles

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Magnetic nanoparticles were synthesized and surface grafted with poly(glycidyl methacrylate) (PGMA) for sensing application. Firstly, magnetite nanoparticles (Fe_3O_4 NP) were synthesized by co-precipitating ferrous and ferric chlorides with ammonium solution. The resultant purified nanoparticles form stable dispersion in ethanol with little aggregation and have a mean hydrodynamic diameter of 151 nm. Transmission electron micrographs (TEM) observe that Fe_3O_4 NP was about 10 – 25 nm in diameter in dried state. The nanoparticles were then surfaced functionalized with α -bromo isobutyryl bromide (BIBB) to form BIB modified magnetite nanoparticles (Fe_3O_4 -BIB NP) with covalent linkage. The resultant Fe_3O_4 -BIB NP is used as a macro-initiator for atom transferred radical polymerization (ATRP) of GMA. The resultant nanoparticles form a very stable dispersion in chloroform with mean hydrodynamic diameters (Z_{ave}) vary from 208 nm to 756nm based on different reaction conditions. Thus, the nanoparticle aggregation during ATRP can be minimized. Aggregates of several primary Fe_3O_4 NPs covered with a thin polymer layer are observed under TEM. Scanning electron micrographs (SEM) show that Fe_3O_4 -PGMA NP can adhere well and distributed on the surface of ultra high molecular weight polyethylene fibres. Vibrating sample magnetometry reveals that the saturation magnetization of original Fe_3O_4 NPs is 66 emu/g and they exhibit superparamagnetism. Upon grafted with PGMA, the value is reduced to 14 emu/g due to the presence of the polymer and the increase of particle size. The high performance fibres coated with polymer functionalized nanoparticles will be embedded into an epoxy matrix for lightweight construction. And the magnetic nanoparticles on the fibres are designed to enable the destruction free diagnostics in polymer-polymer composites.

Multifunctional polymersomes with photoactive moieties and their non-covalent attachment onto surfaces

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Polymersomes have a wide range of biomedical applications such as drug delivery systems¹, synthetic biology or nanoreactors². Interaction between vesicle membrane and their surroundings has played an important role for these applications. Therefore membrane functionalization is a key issue to obtain desired features of the polymersome structure. This study is focused on functionalization of polymersomes with photoactive moieties and adamantane groups. The objective is to obtain light responsive vesicles and their immobilization onto surfaces for targeted carrier systems or biosensors. As a starting point, we synthesized pH sensitive and photo cross-linkable PEG-b-P(DEAEMA-stat-BMA) block copolymers with adamantane and azide end groups to form functional polymersomes. Azide in the structure allows us to attach photoactive moieties to the pre-formed vesicles via click chemistry. As a photoactive moiety, N-nitroveratryloxycarbonyl (NVOC) derivative was used. In this part, amine groups were firstly protected by NVOC photolabile groups then attached to the polymersome periphery. This will give us the opportunity to obtain free amine groups as an additional functionality by irradiating the vesicles at certain wavelengths. This concept will be used to link various biological entities to our vesicles in a controlled manner. Adamantane was used for immobilizing the vesicles onto cyclodextrin modified substrates by using host-guest chemistry. Attachment of polymersomes onto surfaces was confirmed by in-situ AFM in solution at different pH conditions.

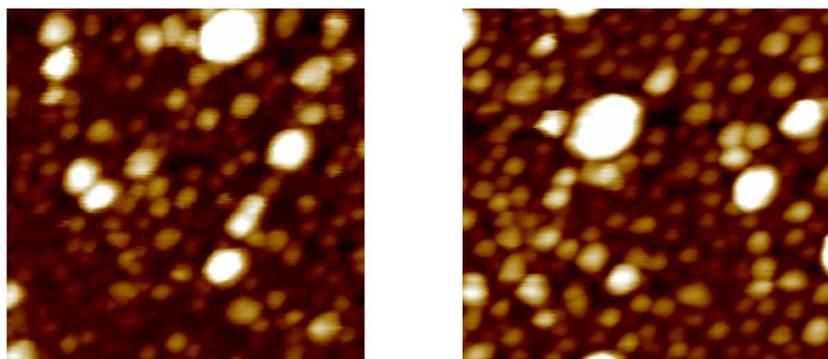


Figure: AFM images of immobilized polymersomes at pH 7.4 (left) and pH 5 (right)

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Elastic Properties of Nickel Carbides

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The nickel -- carbon system has received increased attention over the past years due to the relevance of nickel as a catalyst for carbon nanotube growth and as a substrate for metal-induced crystallization of graphene and graphite. Nickel carbides as bulk materials are out of reach for experimental studies because of their meta-stability. Ab-initio studies are rare. We present our ab-initio -- frozen phonon results for the elastic properties of Ni₃C, Ni₂C and NiC.

Electronic structure of photosensitive molecular switches: A first-principle investigation

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The investigation of networks of nano-particles interconnected with functional molecular components is an active research field. Some potential applications include the realization of elementary computing units, able to act as memory nano-devices. However, to achieve this goal a detailed understanding of the electronic, structural, and electrical transport properties of potentially relevant molecular building blocks is mandatory. Here, we study such properties at the level of single molecules, for merocyanine derivatives, a photosensitive organic complex. In particular, we analyse the interplay between molecular conformation and corresponding modifications in the electrical response.

Surface Patterning and Positioning of DNA Origami on the Nanoscale

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

In the Biomolecular-assembled circuits path, within the excellence cluster “Center for Advancing Electronics Dresden” (cfaed), our goal is to combine top-down with bottom-up strategies to achieve even smaller structures. The circuits will be designed by metalized DNA origamis, but the challenge for this very project is to pattern the Si-based substrate in a way that the DNA will attach specifically and possibly reversibly.

The top-down method of choice is electron beam lithography (EBL). With this technique it is possible to write structures with a resolution down to 5nm. The generated structures are carbon deposits that can be used for further functionalization.

Functionalization will be achieved by self-initiated photografting and photopolymerization (SIPGP). This radical polymerization uses the proton abstraction from the surface that occurs under UV-irradiation with excited vinyl monomers. This generates surface bound radicals that lead to polymer brushes growing from the surface. However, this does not work on bare silicon dioxide surfaces since the SiO-H bonding dissociation energy is too high, but it does on the carbon deposit.

With this difference in functionality it will be possible to precisely tune, not only the position of the DNA on the substrate but also, depending on the used monomer, the binding affinity to the brush.

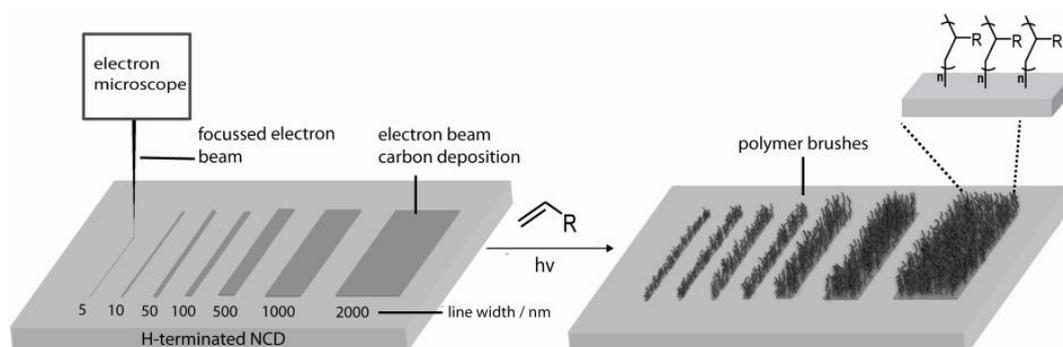


Fig. 1 - Preparation of structured polymer brushes on diamond with electron beam lithography^[1]

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Synthesis of well-defined bis-functionalized semiconducting oligomers for single molecule nanoelectronics

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Tailoring the chemical structure of large delocalized π -systems, which function as bridging components in electronic circuits, is a significant step toward understanding the behavior of single molecules in molecular-scale electronics. A part of this study relies on tuning the electron density of molecular backbone as well as the tunneling of electrons through electrodes in metal-molecule-metal junctions to ensure a general chemical design platform for extracting relationships between molecular structure and electronic properties. The comparison in the optical and electronic properties of semiconducting oligomers having little structural variations is only possible with well-defined molecular chains. For this purpose, Nickel catalyzed Kumada Catalyst-Transfer Polycondensation is utilized for the controlled synthesis of the first generation of thiophene bearing semiconducting oligomers both possessing single/double-sided thiol anchoring groups in different conjugation lengths and different binding positions. Additionally, the effect of using different routes in Kumada and Negishi couplings on tailoring the composition of bis-functionalized oligomers is studied. The optoelectronic properties of oligomers including HOMO-LUMO levels, band gaps as well as their possible alignments on gold surface with respect to their molecular conformations will be investigated. Accordingly, the integration of the oligomers definitely in between two metal electrodes is assured with the exact composition of oligomers and their standing-up phase on gold surface.

Electrical characterization of in-situ switched diarylethene single molecule junctions

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Experimental conductance studies of light-sensitive molecules are presented demonstrating an in-situ change of conductance upon light irradiation. The molecule, photochromic sulfur free diarylethene, is in-situ switched with UV-light in its conductive state. In order to investigate the switching behavior under various conditions, the π -conjugation of the molecular junction is modified with two different side-groups and measured in two different solvents. For the detailed analysis, histograms of conductance traces are taken and complemented by extracting the binding energies and molecular levels from current-voltage characteristics by means of the single-level transport model. The obtained results show a clear controlled light-induced isomerization, almost independent of the side-groups. Furthermore electron-withdrawing side-groups lead to the expected reduction of conductance and strength of the molecular junction.

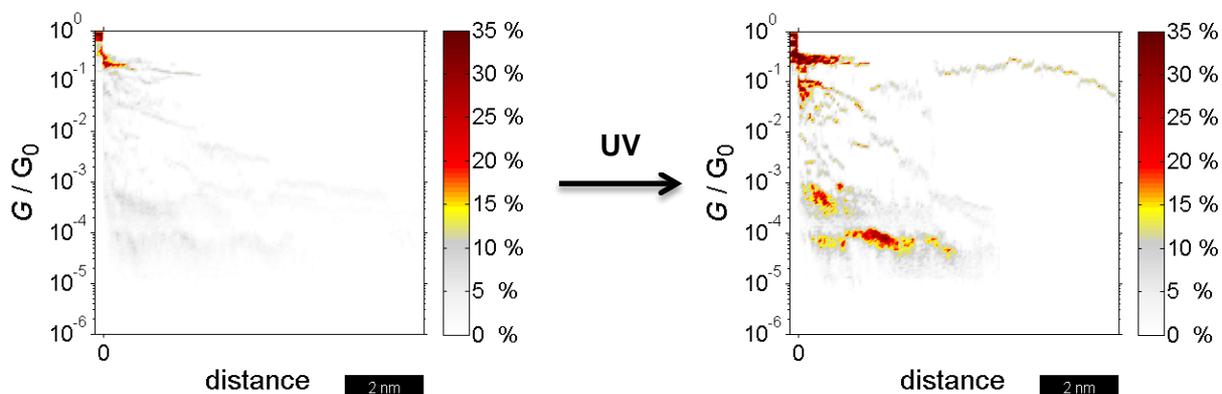


Figure 1. Normalized histograms of conductance traces measured via Mechanically Controllable Break Junction. After in-situ irradiation the non-conductive form of the molecule (left) is switched to the conductive form (right) generating clear plateaus between 10^{-3} and $10^{-5} G_0$.

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Heterogeneous nanoparticle assemblies on DNA Origami

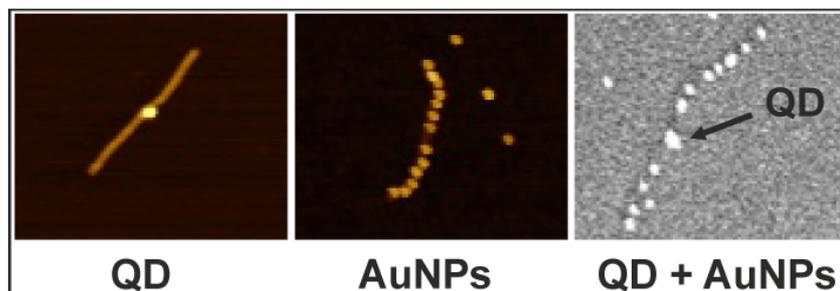
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Nowadays, DNA origami^[1] has become a key technique for designing well-defined nanostructures with any desired shape^[2] and for the controlled arrangement of nanostructures with few nanometer resolution^[3]. These unique features of DNA origami nanostructures make them promising candidates for use as a scaffolds in nanoelectronics^[4] and nanophotonics^[5] device fabrication. In recent years, a number of studies have shown the precise organization of functional nanoparticles on various shapes of DNA origami. Most of these studies used, however, homogeneous nanostructures such as either metallic^[6] or semiconducting nanoparticles^[7]. In this work, we demonstrate the assembly of heterogeneous nanostructures, i.e. 5 nm gold nanoparticles (AuNPs) and 10 nm semiconductor quantum dots (QDs), on a single DNA origami. First, a streptavidin-conjugated QD was assembled on the center of biotin functionalized and immobilized DNA origami nanotube, then DNA coated AuNPs were hybridized along the right and left side of the QD-modified nanotube. The high yield of AuNP assembly was achieved by careful control of the buffer concentration and the hybridization time on Si surface. Our results represent a first step toward the future fabrication of DNA origami-templated quantum dot transistors.



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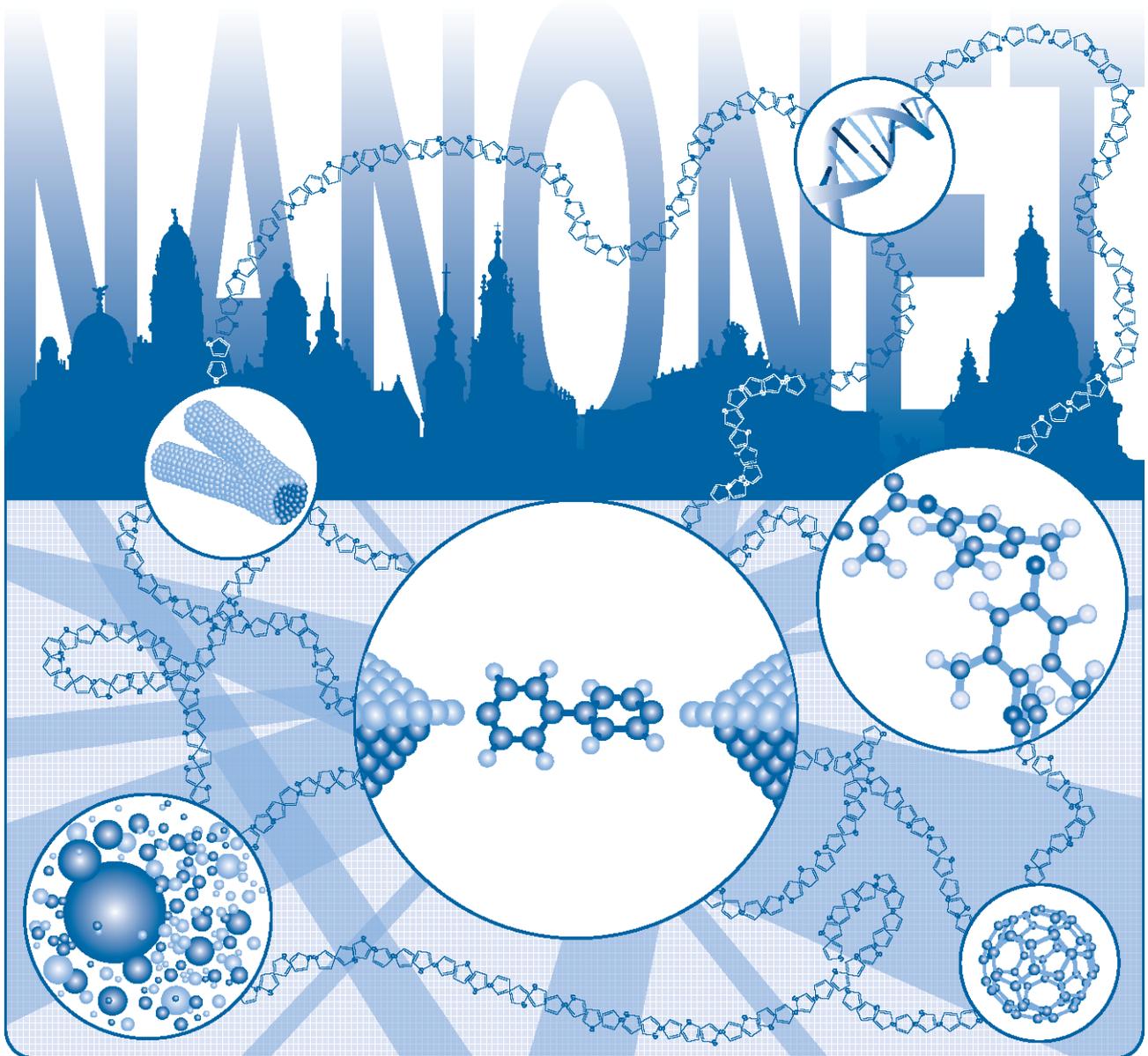
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