International Helmholtz Research School
for Nanoelectronic Networks

HELMHOLTZ ZENTRUM DRESDEN ROSSENDORF

NANONET

IHRS NANONET

Annual Workshop 2020

7 – 9 October 2020

Hotel Friedrichshöhe, Oberbärenburg/Altenberg,

Germany

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HELMHOLTZ RESEARCH FOR GRAND CHALLENGES

NanoNet Annual Workshop 2020 - Altenberg

Agenda

Place: Berghotel Friedrichshöhe, Ahornallee 1, 01816 Altenberg/Oberbärenburg
Web-site: www.hzdr.de/NanoNet-Workshop2020
Updated: 03.10.2020 (PZ)

Wednesday, 7 October 2020

Start	Who	Durat.	Title	Notes
09:09	or 11:09		Bus #360 from **Dresden Hbf** to **Kurort Oberbärenburg**	
12:30			Arrival/Lunch Buffet	
13:30		60	**Coffee + Poster Session (1)**	7 Posters
14:40	Erbe, A.	10	Welcome address	Chair: Erbe
14:50	Blick, R.	40+10	Electron-Spin-Resonance in 2D systems	
15:40		20	**Coffee + Poster Session (2)**	
16:00	Pauly, F.	40+10	Theoretical modeling of photocarrier dynamics in 2D materials & heat transport through molecular junctions	
16:50	Ditte, K.	25+5	Semiconducting organosilicon-based hybrids for the next generation of stretchable electronics	
17:30		60	**Walking Tour – 2.7km - Panorama Tower - View to Dresden**	
19:00			Dinner	

Thursday, 8 October 2020

09:00	Shaygan Nia , A.	40+10	Developing Emerging Two Dimensional (2D) Materials via Electrochemistry	Chair: Fekri
09:50	Arora, H.	25+5	Charge transport in 2D materials and their applications	
10:20		30	Break	
10:50	Schönenberger, C.	40+10	Moiré Superlattice and Strain Engineering of Encapsulated Graphene	Chair: Arora
11:40	Schuster, J.	25+5	Graphene-based nano-laminates - a promising macroscopic conductor material made from nanoscopic building blocks	
12:15			Lunch	
13:45	Dong, R.	30+10	Interfacial synthesis of organic 2D materials: chemistry and function	Chair: Strobel
14:30	Lokamani	15+5	Chain-like assembly of ethoxygroup-functionalized organic molecules on Au(111)	
15:10	Aiboudi, O.	15+5	Molecular Machines: Design, Synthesis and Characterization	
15:30		30	Break	
16:00			**Sightseeing Bob Sledge Run (Tour 16:30)**	
19:00			BBQ	

Friday, 9 October 2020

09:00	Burkard, G.	40+10	Theory of spin qubits and cavity QED in semiconductor nanostructures	Chair: Kilibarda
09:50	Strobel, A.	25+5	Inelastic electron tunneling spectroscopy on Au-C60 junctions	
10:20		30	Break	
10:50	Strunk, C.	40+10	Epitaxial Al/InAs heterostructures as a novel platform for unconventional superconductivity	Chair: Erbe
11:40	Erbe, A.; Zahn, P.	20	Annual Meeting: Status & Future of NanoNet	
12:15			Lunch incl. Student Award Ceremony	
14:00			approx. Departure (Bus #370/360 to Dresden Hauptbahnhof)	

Breakfast will be served from 7:30 a.m.

NanoNet Annual Workshop 2020 - Altenberg

Talks

updated: 03.10.2020 (PZ)

List of Poster Contributions see page **17**.

Electron-Spin-Resonance in 2D-systems

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Graphene has exceptional spin and transport properties, owing to the unique band-structure near the Fermi level. The sublattice-spin is an additional quantum degree of freedom, which couples to the spin, suggesting novel spin manipulation strategies. This promise improvements to high-speed electronic devices and spin-based applications. However, while different theoretical groups disagree on the magnitude of spin and sublattice spin coupling in graphene, little experimental evidence of this coupling exists in literature.
In this work we address the vicinity of the Dirac point by means of low-temperature electron spin resonance (ESR) experiments in electronic transport. This allows us to obtain the necessary low energy resolution to extract a fundamental property of graphene, namely, the intrinsic spin-orbit coupling. We fabricated large chemical vapor deposition (CVD) graphene membranes of 200 µm side lengths and transferred these onto a Si/SiO_2 substrate with a rectangular mechanical modulation of 200 nm pitch and 20 nm height in order to minimize the contact area, and thus interactions, with the substrate. Ohmic contacts were patterned and the sample was mounted next to a coil to generate microwave excitations between spin states. We have detected these electron spin resonances resistively through changes in the sample's longitudinal resistance, R_{xx}. All experiments were performed at liquid helium temperature of 4.2 K and magnetic fields of up to 8 T.
In addition to the regular electron Zeeman splitting, the ESR experiments reveal a zero-field splitting, which will be discussed in my presentation. This value has been also reported in earlier studies with different substrate materials, sample geometry and graphene quality. This robustness reflects the intrinsic and microscopic nature of this coupling, mainly due to the d-orbitals in graphene.

Theory of spin qubits and cavity QED in semiconductor nanostructures

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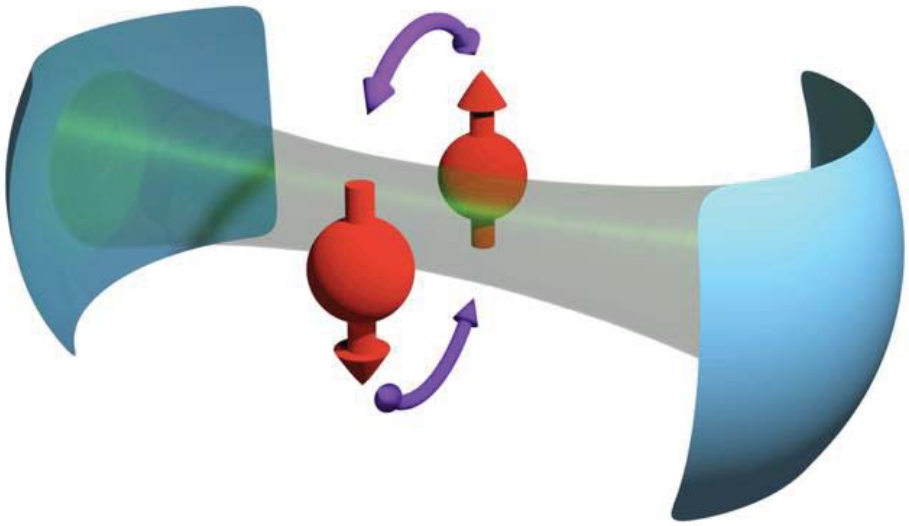
This talk will highlight recent advances related to spin-based quantum information processing from a theoretical perspective, including the impact of new material systems and nanostructures, electric spin control, and the coupling of individual spins to the quantized field of a superconducting microwave resonator (see [1] for a recent review article). We discuss the importance of spin-charge hybridization for spin qubit control and measurement, and present several examples. Recently, electric spin control using synthetic spin-orbit coupling due to magnetic field gradients in combination with the exchange coupling has allowed for electrically controlled one- and two-qubit gates for spins in silicon quantum dots. An alternative approach to all-electric control of spin qubits consists in the use of multi-spin qubits containing more than one electron, such as the singlet-triplet, exchange-only, and resonant-exchange qubits (see [2] for a review), as well as quadrupolar qubits. The development of superconducting coplanar waveguide resonators has provided new opportunities for coupling spin qubits over long distances which have come into the reach of experimental feasibility with the recent achievement of the strong-coupling regime in spin-cavity quantum electrodynamics (QED).



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Interfacial Synthesis of Organic 2D Materials: Chemistry and Function

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Abstract

The discovery of graphene one decade ago has triggered enormous interest in developing chemistry of synthetic two-dimensional materials (2DMs). In our work, we have employed molecular design and interfacial chemistry toward the controlled synthesis of organic 2DMs with diverse structures and functions.[1] For instance, in our early work, we demonstrated the synthesis of 2D conjugated metal-organic framework (2D *c*-MOF) at the air-water or liquid-liquid interfaces.[2] The 2D *c*-MOFs feature with stacked layers and possess unique electronic properties, such as full π delocalization, narrowed band gaps, high conductivity and high mobility, which render 2D *c*-MOFs as advanced electronic materials for MOFtronics. One representative iron-bis(dithiolene) 2D MOF exhibited as a *p*-type semiconductor with a band-like transport and record mobility of ~220 cm^2/Vs.[2a] Owing to their conductivity, the 2D *c*-MOFs have shown potential for transistors, photodetectors, sensing, magnetics, and energy storage and conversion.[1,2a,3,4] In addition, we have also synthesized conjugated 2D covalent polymers at the air-water or liquid-liquid interfaces.[1] In our latest work, we have employed a surfactant-monolayer-assisted interfacial synthesis (SMAIS) method to prepare 2D polymers, like 2D polyimides and 2D polyimines, which exhibited few-layers and micrometer-sized single-crystalline domains and were utilized for transistors and memory devices.[5] In short, we expect to develop controlled synthesis of organic 2DMs and achieve delineation of reliable structure-property relationships and superior physical and chemical performances of organic 2DMs.

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Theoretical modeling of photocarrier dynamics in 2D materials & heat transport through molecular junctions

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This presentation is split into two parts. In the first one, I will speak about the dynamics of photoexcited charge carriers in two dimensional materials. The second is devoted to heat transport through nanostructures, in particular through molecular contacts.

- Utilizing high-energy carriers in photovoltaic devices could improve light-to-energy conversion efficiencies. To achieve this goal, hot-electron transfer between active and passive layers should be facilitated or photocarrier lifetimes extended. Van der Waals (vdW) semiconductor heterostructures formed from atomically thin two-dimensional (2D) crystals might represent a suitable platform to take advantage of both phenomena. I will describe our parameter-free ab initio modeling of photocarrier thermalization due to electron-phonon interactions [1-3]. Based on it, I will study the photocarrier thermalization bottleneck in graphene [1], the impact of spin-orbit splitting on the thermalization behavior in transition metal dichalcogenides and the internal quantum efficiency of van der Waals heterostructures [2], as well as the differences in charge carrier thermalization in bulk and monolayer CdTe [3]. If time permits, I will shortly discuss recent experiment-theory investigations of excitonic processes [4,5].
- Single-atom and single-molecule junctions turn out to be ideal platforms for testing quantum theories that are required to describe charge and energy transport in novel nanoscale devices. However, the thermal conductance of single-molecule junctions has not been determined directly until recently, owing to the challenge of detecting minute heat currents at the picowatt level. In this part, I will discuss how picowatt-resolution scanning probes, previously developed to study the thermal conductance of single-metal-atom junctions [6-8], allow to measure the thermal conductance of single-molecule junctions [9]. Using prototypical Au-alkanedithiol-Au junctions containing 2 to 10 carbon atoms, I will discuss the comparison of experimental results with our present theoretical understanding based on first principles and molecular dynamics computational modeling [9-12].

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Moiré Superlattice and Strain Engineering of Encapsulated Graphene

(alphabetic order) G. Abulizi[1], A. Baumgartner[1], D. Indolese[1], P. Makk[1,2], C. Schönenberger[1,3,*], T. Taniguchi[4], L. Wang[1], K. Wanatabe[5], S. Zihlmann[1]

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Moiré superlattices in van der Waal's stacked two-dimensional (2D) materials receive a large attention now. This was fueled by the remarkable observation of superconductivity in twisted bilayer with small twist angles and therefore large superlattice unit cells. I will show how superlattices appear in different kind of measurements of h-BN encapsulated graphene aligned to h-BN and that it is possible to induce a "double Moiré", when the graphene layer is aligned with both the bottom and top h-BN. Further on, I will introduce a new technique and sample design allowing to engineer strain in fully h-BN encapsulated graphene, avoiding valley mixing due to disorder while straining. We show that strain and strain gradients can be deterministically generated. We then analyze the effect of strain on various transport phenomena, such as carrier mobility, conductance fluctuations, transverse magnetic focusing and Landau quantization, and critically discuss their origin based on both strain-induced scalar potential and pseudo-magnetic field. It is believed that strain is a key parameter to understand domain formation in the stacked 2D materials.

Developing Emerging Two Dimensional (2D) Materials via Electrochemistry

Ali Shaygan Nia[1], Huanhuan Shi[1], Panpan Zhang[1], Sheng Yang[1,2] and Xinliang Feng*[1]

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2D materials are important building blocks for the next generation of electronic and energy devices due to their remarkable chemical and physical characteristics. To this end, large-scale production of 2D materials with high purity and with specific functionalities represents a key to advancing fundamental studies as well as industrial applications. Among different synthetic protocols, electrochemical exfoliation[1] of layered materials is a very promising approach that offers high yield, great efficiency, low cost, simple instrumentation, and excellent up-scalability. Remarkably, playing with electrochemical parameters not only enables functionalization and tunable material properties but also increases the material diversities from graphene to a wide spectrum of 2D semiconductors[2].

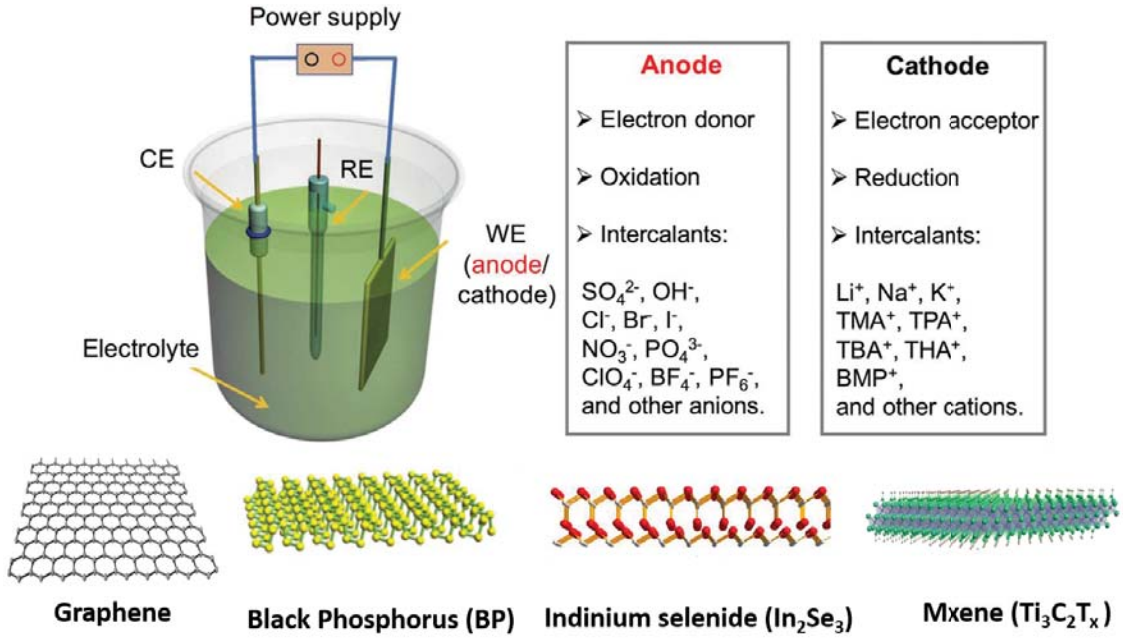

Figure 1. Schematic illustration of electrochemical exfoliation methodology and different 2D materials which could be produced *via* this method

References:

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Epitaxial Al/InAs heterostructures as a novel platform for unconventional superconductivity

Christoph Strunk

Regensburg University

Rashba-type spin orbit interactions break inversion symmetry and lead to the relatively new class of non-centrosymmetric superconductors. We employ inductance measurements to investigate the supercurrent response in one-dimensional Josephson junction arrays and long strips patterned into an epitaxial Al/InAs-heterostructure. The Josephson inductance provides a deep insight into the properties of our ballistic junctions: we observe a very high average transparency (up to 94%) of our ballistic junctions, determine the number of highly transmissive channels, and extract the induced gap within the InAs quantum well underneath the Al film. In a parallel magnetic field time-reversal is broken in addition to inversion symmetry. This leads to an interesting magneto-electric asymmetry of the junctions: critical current and Josephson inductance develop a diode-like behavior, i.e., they depend on the sign of both the current and the parallel field.
Also superconductivity in plain 2d heterostructures turns out to be strongly affected by SOI. In a parallel magnetic field superfluid stiffness and vortex pinning become strongly anisotropic with respect to the angle between field and current direction. The vortex pinning strength is greatly enhanced by the parallel field. Such behavior is considered as a hallmark of unconventional pairing.

Design, Synthesis and Characterization of an Azulene Based Nanocar on Gold

Oumaima Aiboudi[1,2]

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Miniaturizing motors and machines down to nanometer scales could lead to a new industrial revolution but realizing such designs remains a challenge. Inspired by macroscopic machine counterparts, several types of molecular machines, such as nanoscale shuttles,[1] nanorotors,[2] and nanovehicles[3] have been synthesized. Among these, we focused on the synthesis of nanocars that are able to convert external electrical energy into controllable translational motion on gold surfaces.

The dipole moment was reported to enable controlled movements by voltage pulses. We targeted 2-isocyano-1,3-di-*tert*-butyloxycarbonyl azulene. The dipole moment of unsubstituted azulene is 1.08 D. Introducing suitable push/pull substituents allows to achieve dipole moments up to the range of 10 D. We hypothesized that the azulene core would act as a dipolar motor and respond well to the external electrical field of the STM tip, allowing to move the nanocar. Both isonitrile and ester substituents at the chosen positions heighten the dipole moment of the azulene. The two *tert*-butyl ester groups avoid a fully planar structure and raise the azulene core above the surface. The synthesis of the target compound was achieved in four steps, with an overall yield of 70%.

The azulene-based nanocar was fully characterized physico-chemically, and then investigated on a gold surface under low-temperature UHV conditions to study the role of dipole moment and charge distribution on lateral movement. STM investigations and simulations revealed the formation of several dimeric structures *via* the coordination to an adatom on the gold surface, while single molecules were very scarce. Of three observed nanostructures those with high molecular dipole moments of 9 D and 6.5 D, can not be moved efficiently. On the other hand, a dimer with a much lower dipole moment of 2.3 D can be controllably driven on the surface Based on this we assume that the dipole moment is of minor importance in the voltage-pulse induced molecular manipulation compared to the charge distribution. The clear dependence of the threshold voltage for lateral movement on the electric field demonstrates that the charge separation in the structure plays a major role.

For our next nanocar design, we will mainly focus on the synthesis of charged molecules (e.g. DMBI) as a molecular motor.

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Charge transport in two-dimensional materials

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

In the second part, electronic and opto-electronic properties of a novel 2D semiconducting metal-organic framework (MOF) with the formula $Fe_3(THT)_2(NH_4)_3$ (THT=2,3,6,7,10,11-hexathioltriphenylene) are discussed. We demonstrate for the first time band-like charge transport in MOFs using Hall-effect measurements. A record mobility of 230 $cm^2V^{-1}s^{-1}$ at room temperature is obtained in 1.7 µm thick MOF films. Subsequently, proof-of-concept photodetectors are fabricated with $Fe_3(THT)_2(NH_4)_3$ as an active element. The photodetectors demonstrate broadband photodetection in UV–NIR region, in addition, show a stable and reproducible photoswitching characteristics.

Semiconducting organosilicon-based hybrids for the next generation of stretchable electronics

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Polymer semiconductors (PSCs) are an essential component of organic field effect transistors (OFETs), but their potential for stretchable electronics is limited by their brittleness and failure susceptibility upon strain. Recently, research has focused on enhancing their stretchability by utilizing different (molecular) engineering approaches. Here, we demonstrate a new synthetic design strategy: triblock copolymer (TBC) structures are realized by covalently connecting semiconducting poly-diketo-pyrrolopyrrole-thienothiophene (PDPP-TT) and elastomeric polydimethylsiloxanes (PDMS). This approach allows the segregation of two phases while preserving the respective properties of the individual polymers, i.e. high charge carrier mobility and mechanical compliance, in one system. TBCs containing up to 65 wt.-% PDMS were obtained, and the TBC with 65 wt.-% PDMS content exhibits mobilities up to 0.1 $cm^2V^{-1}s^{-1}$, in the range of the fully conjugated reference polymer PDPP-TT (0.7 $cm^2V^{-1}s^{-1}$). The TBC is ultra-soft with a low elastic modulus ($5x10^6$ Pa) in the range of mammalian tissue. Conductivity, elastic constants and PDMS content are thus beyond values possible for physical blends of the two polymers. Furthermore, the TBC is stretchable without crack formation up to 85% strain, and is extraordinarily durable, maintaining electronic functionality at different applied strain levels **(0, 50, and 100 %)** after 1000 cycles to 100% strain.

Chain-like assembly of ethoxygroup-functionalized organic molecules on Au(111)

Lokamani[1,2,3], Jeffrey Kelling[3], Robin Ohmann[1,4], Jörg Meyer[1], Tim Kühne[5], Gianaurelio Cuniberti[1], Jannic Wolf[6], Thomas Huhn[6], Peter Zahn[2], Francesca Moresco[5], and Sibylle Gemming[2,7]

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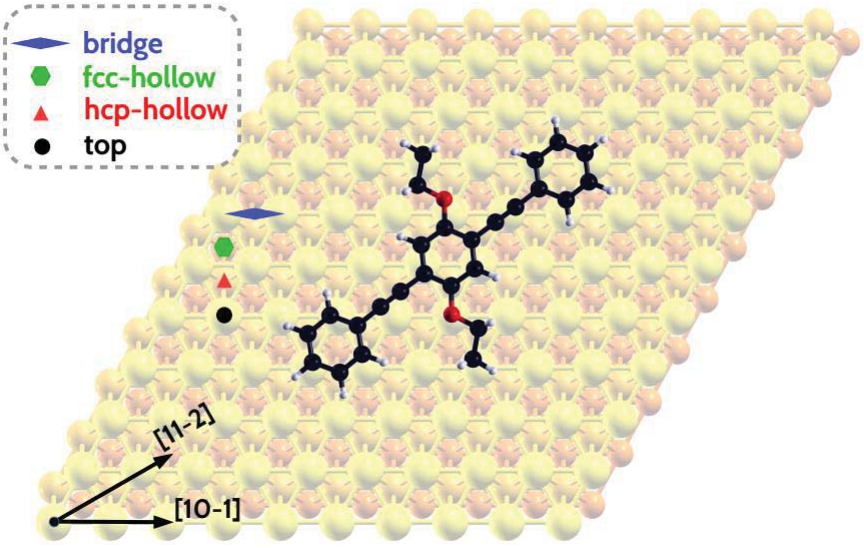
The electronic and geometrical structure of 1,4-bis(phenylethynyl)-2,5-bis(ethoxy)benzene (PEEB) molecules adsorbed on a Au(111) surface is investigated by low temperature scanning tunneling microscopy (STM) and scanning tunneling spectroscopy in conjunction with density functional theory tight-binding (DFTB) simulations of the density of states, the interaction with the substrate and the intermolecular interactions. Our density functional theory calculations indicate that the PEEB molecule is physisorbed on the Au(111) substrate, with negligible distortion of the molecular geometry and charge transfer between molecule and substrate. Additionally, due to the low corrugation of the Au(111) surface, PEEB molecules can form quasi interlocked lateral patterns, which are observed in STM experiments. In order to explain the interlocked lateral patterns, we employ DFTB+ -based high-throughput calculations including universal force field for dispersion corrections to evaluate an energy function which incorporates the adsorption energy of single PEEB molecules on the metal surface and the intermolecular interaction energy of a pair of PEEB molecules. The analysis of the energy function reveals, that, depending on coverage density, specific types of pattern are preferred which can potentially be exploited to form one-dimensional molecular wires on Au(111).



Graphene-based nano-laminates – a promising macroscopic conductor material made from nanoscopic building blocks

Jörg Schuster[1,2], Leo Rizzi[2,3], Martin Koehne[3], Stefan E. Schulz[1,2]

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Graphene nano-laminates (GNL) consist of disordered stacked sheets of pure graphene, which form a macroscopic material. They are fabricated from suspensions of graphene or graphene oxide. GNLs can be prepared as films or can be spun into fibers. The material is flexible, strong, and lightweight. After reduction, doping and thermal treatment GNLs can reach very high electrical conductivities of several tens of MS/m. Thus, they have the potential to be a lightweight alternative to metals in many application fields.

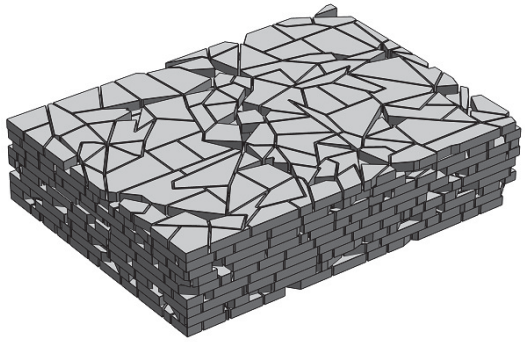

Figure 1: Schematic view of the GNL model

Based on a statistical network simulation model [1] we analyze the potential of GNLs systematically. For this purpose, we model large systems of randomly arranged graphene flakes. In our model, the flakes may have arbitrary size and shape. By checking all interconnections between the flakes, we transform the system of flakes into a resistor network, which is solved afterwards. Besides the geometrical parameters like size, shape, orientation and packing density, we consider the in-plane conductivity within a flake and the out-of-plane conductivity between overlapping flakes. By averaging over many configurations of flakes, we calculate the total conductivity of the system as a function of all parameters.

The results of our simulations show clearly, that out-of-plane conductivity and flake size are the key factors to reach a highly conductive macroscopic material [2]. Only for GNLs consisting of large flakes of several tens of microns and good out-of-plane conductivities, we can transfer the excellent conductivity of the single graphene flakes to the macroscopic conductivity.

In order to check our models, GNL-films consisting of size selected graphene flakes have been prepared and analyzed carefully [3]. As simulation and experiments are in a perfect agreement, we conclude that our microstructural model is valid and provides a solid basis for a systematic optimization of graphene nano-laminates towards metallic conductivity.

[1] L. Rizzi, J. Schuster, et al.; Comp. Mat. Science 161 (2019), p. 364
[2] L. Rizzi, J. Schuster, et al.; ACS Appl. Mater. Interfaces 10 (2018), p. 43088
[3] L. Rizzi, J. Schuster, et al.; Nano Express 1 (2020), p. 020035

Inelastic electron tunneling spectroscopy on Au-C60 junctions

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Current industrial semiconductor scaling processes are reaching limits. We see not only diminished returns with further scaling attempts, but also physical limitations that come more and more into play. In our research we offer a novel approach, where we try to drop altogether the concept of 3D scaling of electronic components and go to practically 1D molecular systems. This approach offers not only reduction in power consumption and costs, but also a deeper understanding of the electron transport behavior of molecules. Our research focuses on classifying different molecules with the help of Mechanically Controlled Break Junction (MCBJ) technique.

The talk focuses on C_{60} Fullerenes using a unique low-temperature MCBJ setup. Fullerenes are considered mediator for the Bonding between electrodes (Au) and molecule. The setup enables to thermally evaporate Fullerenes *in situ* and perform measurements under high vacuum conditions. Electron-phonon interaction and the corresponding inelastic tunneling spectra can serve as the molecules' fingerprint. These spectra along with differential conductance- and the voltage-current-characteristics were simultaneously measured. Results for different Conductance regimes are discussed.

Your Notes

NanoNet Annual Workshop 2020 - Altenberg

Posters

updated: 03.10.2020 (PZ)

1) Posters can be mounted on arrival. The posters should be on display the whole time.
2) Please, remove your poster latest on Friday noon.

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

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

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Quantum mechanical band-to-band tunneling (BTBT) is a particular type of carrier injection mechanism which is responsible for the electronic transport in tunneling based devices like Esaki diode and Tunnel Field Effect Transistor (TFET)[1][2]. Atomically thin layers of transition metal dichalcogenides (TMDCs) are promising semiconducting materials for realizing such devices owing to their sharp interfaces. We demonstrate BTBT between the layers of molybdenum disulfide (MoS2) and tungsten diselenide (WSe2) in a MoS2-WSe2 heterojunction which is encapsulated with hexagonal boron nitride (h-BN) on the top and bottom. Also, we employ few-layer graphene as the contact material to the heterojunction thereby forming a 2D-2D van der Waals contact. We observe negative transconductance and negative differential resistance in the fabricated device thereby indicating the tunnelling behaviour.

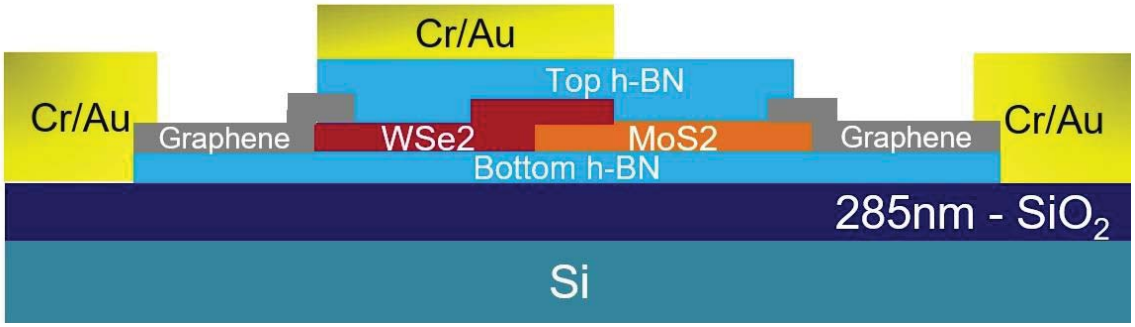

Figure 1: Schematic of the fabricated device

References

[1] Amirhasan Nourbakhsh, Ahmad Zubair, Mildred S. Dresselhaus, and Tomás Palacios, Nano Letters, 2016, 16(2):1359–1366.

[2] Tania Roy, Mahmut Tosun, Xi Cao, Hui Fang, Der-Hsien Lien , Peida Zhao, Yu-Ze Chen, Yu-Lun Chueh, Jing Guo, and Ali Javey. *Acs Nano*, 2015, 9(2):2071–2079.

Hall bar configuration for characterisation of highly doped Ge nanowires

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Germanium (Ge) is a promising high mobility channel material for future nanoelectronics that can offer an improved performance at reduced power consumption compared to Si electronics. Despite the improvement of semiconductor nanowires (NWs) research, doping and characterising the electrical properties of NWs remains a challenging task. The most widely used electrical characterisation method, field effect (FE) mobility measurements, is relatively simple in terms of device fabrication and measurements. However, the accuracy is questionable, and therefore, careful methodology is necessary in order to properly estimate the gate capacitance and account for contact resistance. On the other hand, Hall effect measurements enable a more precise characterisation of the carrier concentration and mobility of NWs and do not rely on estimations of critical input parameters.

In this context, highly p-doped Ge nanowires were fabricated using electron beam lithography and inductively coupled plasma etching. Subsequently, we carry out the Hall effect measurement for a single Ge NW using six-contact Hall bar configuration to minimise the geometrical source errors. Furthermore, this configuration can be used for a four-probe electrical measurement. The carrier concentration, carrier mobility and the resistivity of Ge NWs with different widths were measured using this configuration.

Simulation of $NiSi_2$-Si Interfaces: Stability, Schottky Barriers, and Tunneling Transport

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The influence of strain on the stability and the transport properties of $NiSi_2$−Si interfaces is studied using density functional theory and atomistic quantum transport simulations. All relevant crystal orientations are investigated in the strain range of ±2%.
We show that the response of the electron and hole tunneling currents upon deformation is strongly orientation dependent. The {110} interface enables symmetric electron and hole currents under specific strain conditions. The {110} interface, however, is less stable than the {111} interface, which is often observed experimentally in ⟨110⟩ nanowires [1]. Based on geometrical considerations, we suggest that reducing the diameter could allow control of the interface [2].
Furthermore, two more simplified models are used to understand the underlying physics of the $NiSi_2$−Si interface. The first applies the Wentzel-Kramers-Brillouin and the triangular barrier approximations to calculate tunneling currents. This model reproduces general trends, but deviates whenever the shape of the barrier deviates from the triangular barrier. The second model is the metal-induced gap states model, which is used to relate the Schottky barrier height to the work functions of the separated materials.

[1] Khan et al., *Appl. Sci.* **9**, 3462 (2019)
[2] Fuchs et al., *J. Appl. Phys* **128**, 085301 (2020)

Homocoupling Defects in Donor-Acceptor Polymers

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Homocoupling defects in semiconducting conjugated polymers have been discussed to deteriorate the structural and electronic properties of the semiconductor material and thus of the device performance. To ensure batch-to-batch reproducibility of functional elements based on DA polymers control over structural deviations from the regular D-A sequence has thus been a major goal for synthesis. The present study investigates homocoupling (hc) defects in copolymers made from dithiazolyldiketopyrrolopyrrole (TzDPPTz) and tetrafluorobenzene (F4) by direct arylation polycondensation (DAP). TzDPPTz hc defects in the resulting copolymers **PTzDPPTzF4** are correlated with several reaction parameters and can be quantified experimentally. The effect of hc density on the optical, morphological and electronic properties of **PTzDPPTzF4** is investigated by density-functional-based tight-binding calculations. While TzDPPTZ hc defects cause red-shifts of the absorption spectra, the morphology and field-effect mobility in organic field-effect transistors are marginally or not affected. In-line with preliminary experimental observations, hc content is not limiting device performance for **PTzDPPTzF4** copolymers.

Fabrication of dual gated reconfigurable devices with controlled nickel silicidation

Bilal M. Khan, HZDR

To complement the scaling down of CMOS, new device concepts have been introduced. One of these concepts is reconfigurable field effect transistors (RFETs) which is based on undoped silicon nanowire (SiNW). SiNWs are nickel silicided at both ends, yielding silicide-Si-silicide Schottky junctions. Two distinct gate electrodes are fabricated on these junctions. By controlling the electrostatic potential on the gate electrodes, the RFET is programmed to *p*- or *n*- polarity. We report on the fabrication and electrical characterization of top-down fabricated RFETs. Flash lamp annealing is used for silicidation instead of rapid thermal annealing to enable control over the silicidation process.

Temporal evolution of molecular junctions formed in MCBJ experiments

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The general approach to quantify molecular behavior is to characterize junction distance dependence under constant voltage. Subsequently, if we observe the formation of molecular steps, we can further explore their properties with the voltage sweeps. We can then extract the underlying parameters by fitting to the single level model (SLM). Finally, to present the data, we plot these parameters on histograms and explore newly present features. This approach gives only the averaged behavior of molecules in the junctions and does not say anything about how parameters depend on the distance and the conditions present.
Here we will present a complementary approach by exploring the temporal evolution of the SLM parameters.
As a result, we will suggest possible interpretations of the molecular binding and how molecular behavior depends on the binding position.

Nano-electronic components built from DNA templates

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On the nanoscale, fundamental properties and potential applications are greatly influenced by the size and shape of the material. “DNA Origami” takes advantage of base complementarity of individual short oligonucleotides, to fold a long “scaffold strand” into almost any continuous 2D or 3D shape.[1] We introduced a new concept of DNA origami mold-based particle synthesis that allows the synthesis of inorganic nanoparticles with programmable shape. We demonstrated the concept by fabricating a 40 nm long rod-like gold nanostructure with a quadratic cross-section.[2] We expanded the capabilities of the mold-based particle synthesis to demonstrate the synthesis of uniform µm long conductive gold nanowires with 20-30 nm diameters.[3] With conductance characterization, metallic conducting wires were demonstrated. Here the concept is further expanded by designing mold monomers with different geometries and interfaces. We can fabricate more complex ‘mold-superstructure’ in a unique and flexible way based on this modular DNA platform (see figure 1).[4,5] We can also incorporate semi-conducting nano-rods into this mold-based system for further single molecular transistor application.[6] In addition, double-stranded DNA layer known for high spin-selectivity, incorporated in the metallic wire can also be used as efficient spin filter for spintronic applications.

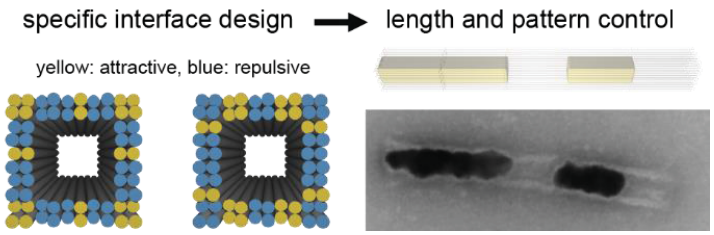
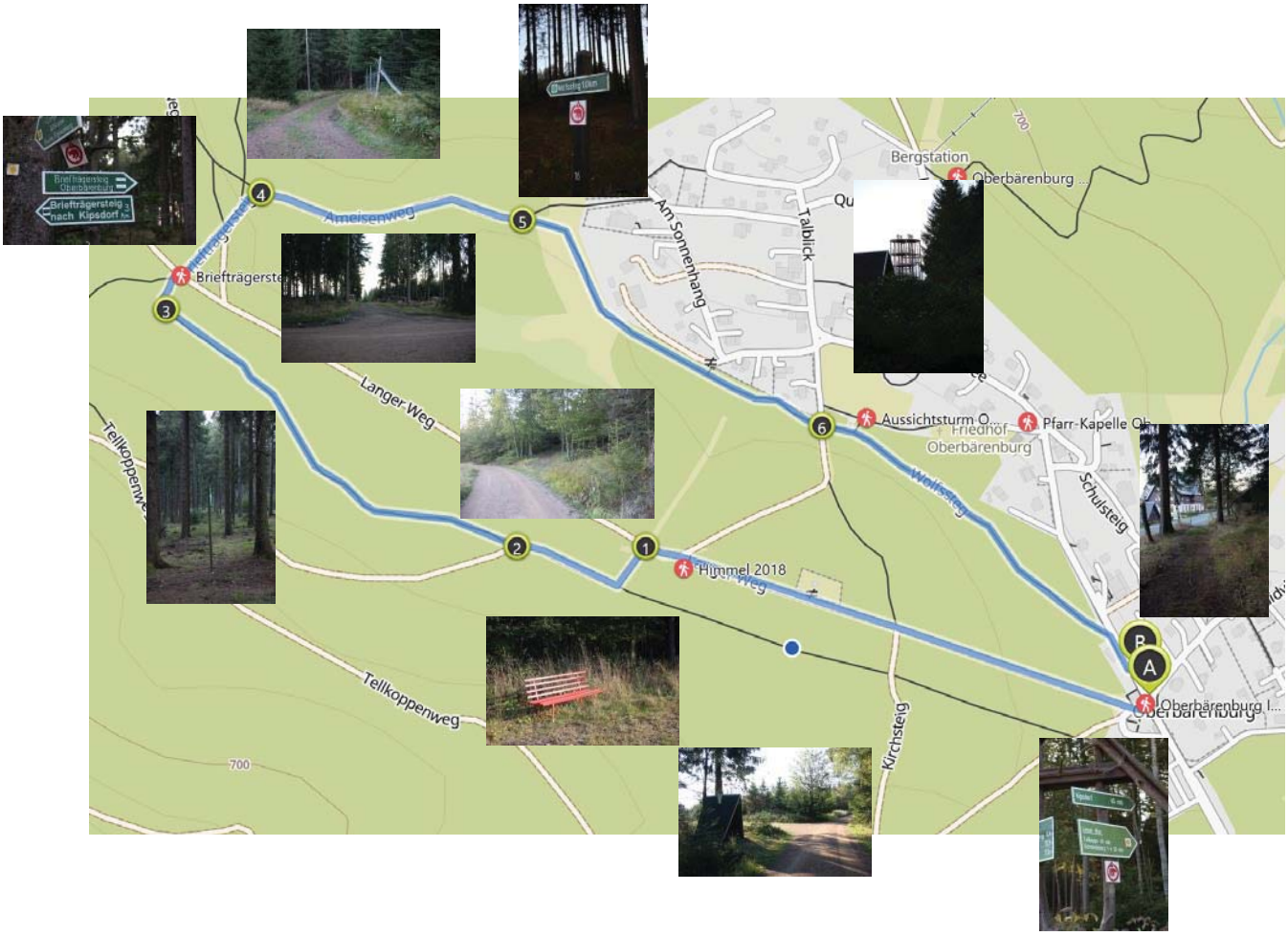


Figure 1. Sketch and tSEM images showing the modular DNA platform. With specific interface design by choosing different helix positions for attractive and repulsive reaction, the length and pattern of the metal structures can be controlled.

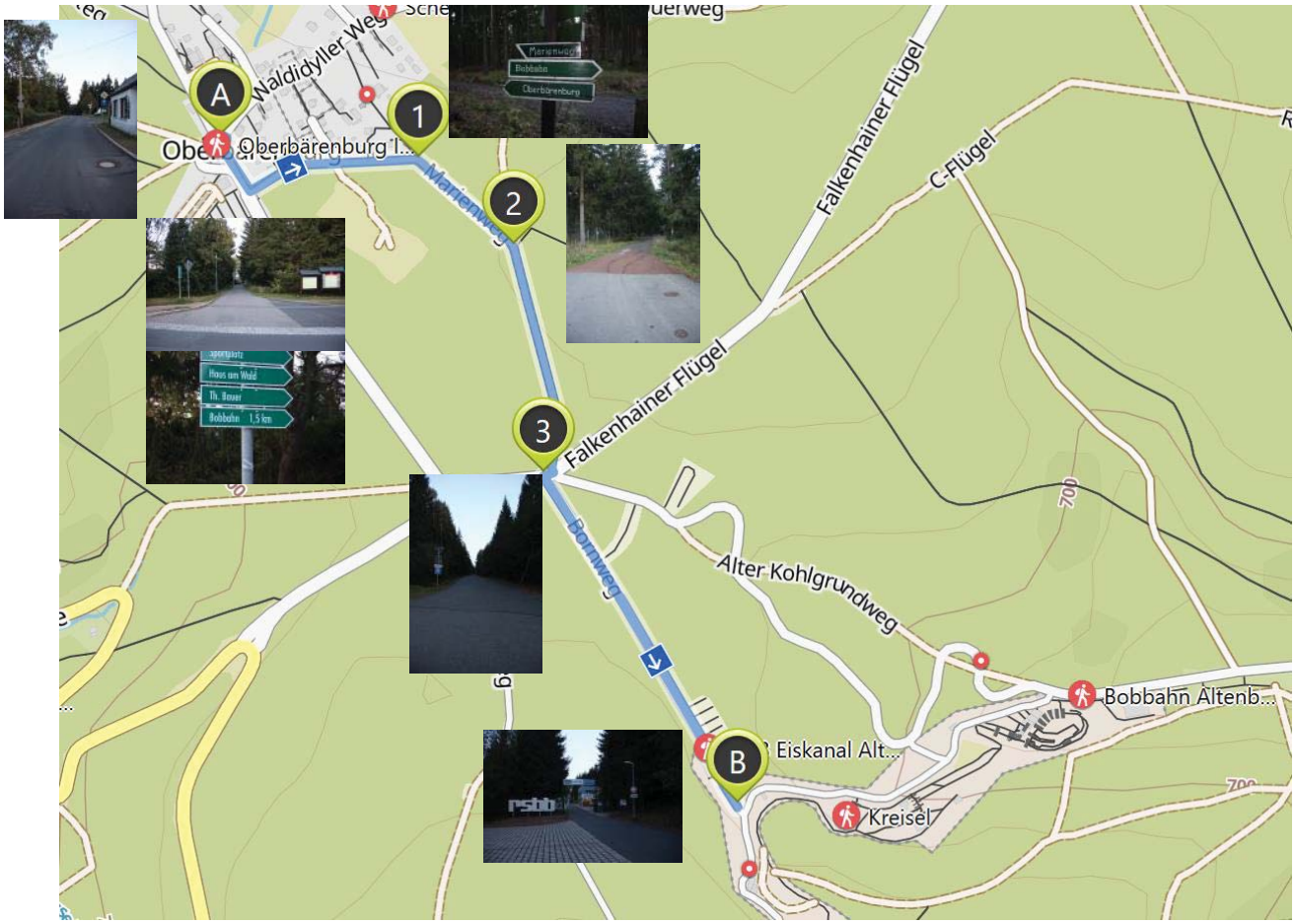
(1) Rothemund, P. W. K. *Nature* **2006**, *440* (7082), 297–302.
(2) Helmi, S.; Ziegler, C.; Kauert, D. J.; Seidel, R. *Nano Lett.* **2014**, *14* (11), 6693–6698.
(3) Bayrak, T.; Helmi, S.; Ye, J.; Kauert, D.; Kelling, J.; Schönherr, T.; Weichelt, R.; Erbe, A.; Seidel, R. *Nano Letters* **2018**, *18* (3), 2116–2123.
(4) Ye, J.; Helmi, S.; Teske, J.; Seidel, R. *Nano Lett.* **2019**, *19* (4), 2707–2714.
(5) Ye, J.; Weichelt, R.; Kemper, U.; Gupta, V.; König, T. A. F.; Eychmüller, A.; Seidel, R. *Small* ***2020***, 2003662.
(6) Weichelt, R.; Ye, J.; Banin, U.; Eychmüller, A.; Seidel, R. *Chemistry – A European Journal* **2019**, *25* (38), 9012–9016.

Your Notes

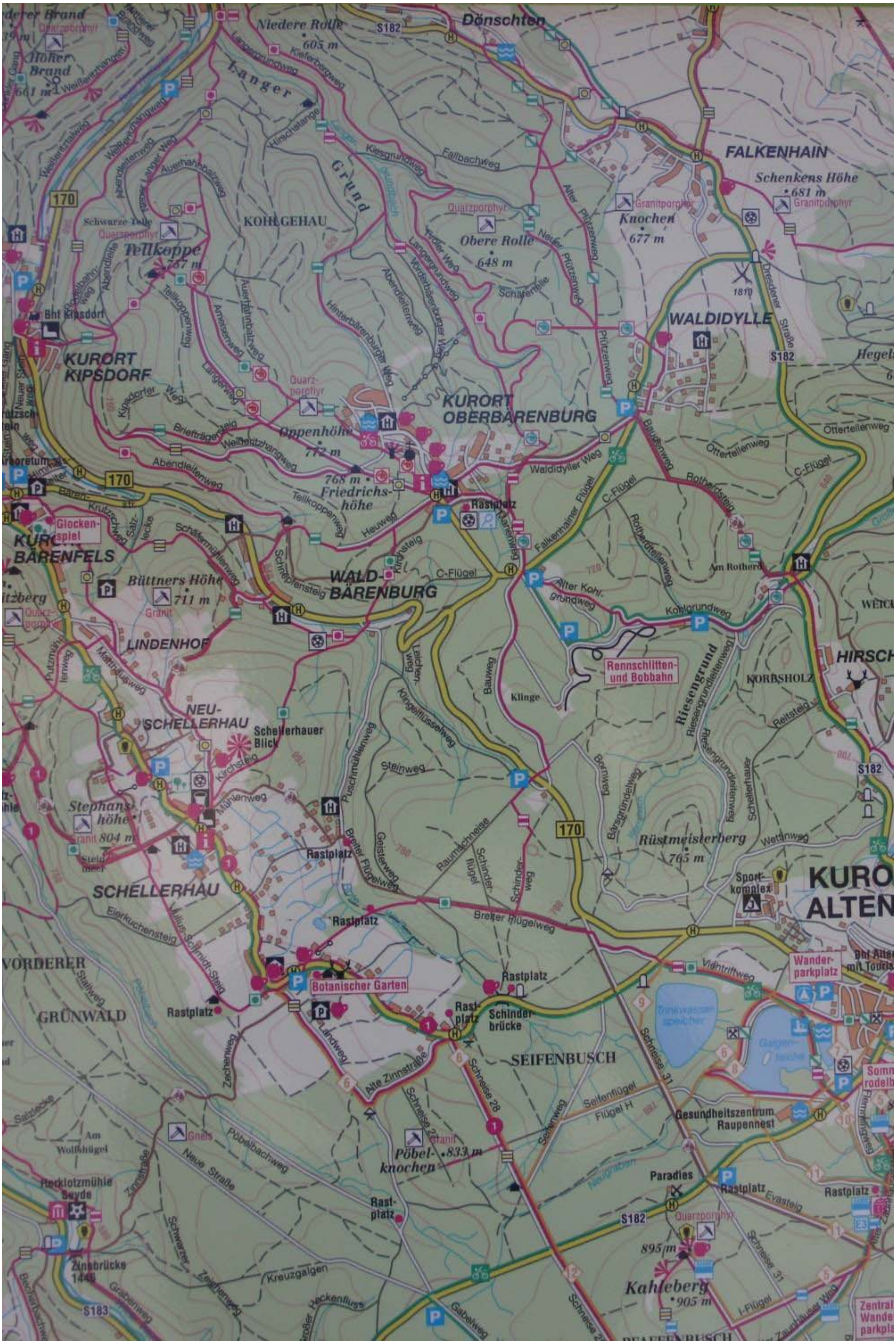
Hiking Tour to **Schellerhau Blick and Panorama Tour** (total 2.7km, 1h, Wed)
A: Hotel Friedrichshöhe,
1: turn to the left, reach the View to Schellerhau after 100m (red bench)
2: turn a bit right in a smaller path, follow this
3: turn right at a larger path, cross a forest road, follow **Briefträgersteig**
4: follow the right turn,
5: turn right in the small path- a bit upwards,
6: the Panorama Tower, in direction North you may identify Dresden area, follow then the small path in the forest (Wolfssteig) or the small street along the Chapel,
B: You reached the dinner site.



Walk to **Bobbahn Altenberg** (one direction 1.5km, 25 min., Thu)
A: Hotel Friedrichshöhe, go to the bus stop, then turn left into **Marienweg**
1: turn slightly right,
2: turn slightly right again,
3: cross the main road, follow the asphalt path
B: You reached the meeting point for the Guided Tour.
After the guided tour we return on the same way- a small light be nice, but is not mandatory.



Map of the Area



NanoNet Annual Workshop 2020 - Altenberg

Participants (partially on-line)

Updated: 03.10.2020 (PZ)

Name	First Name	Gender	Title	Institution
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