8 PhD positions at the International Helmholtz Research School for Nanoelectronic Networks (IHRS NANONET)

The International Helmholtz Research School for Nanoelectronic Networks (IHRS NANONET) is an initiative of the Hemholtz-Zentrum Dresden - Rossendorf (HZDR) in a joint collaboration with the Technische Universität Dresden (TUD), Leibniz Institut für Polymerforschung Dresden e.V. (IPF), Fraunhofer Institute for Ceramics Technologies and Systems IKTS-MD, and the Nanoelectronics Materials Laboratory (NaMLab) gGmbH. The research School offers an interdisciplinary research training program in the field of **molecular electronics**. The 3-year PhD programme includes independent research work in a project involving different divisions of science and engineering and a well-structured scientific curriculum providing for a comprehensive training in technical and professional skills.

8 PhD positions are now available within the IHRS NANONET located at the participating institutions. For a detailed description of the project objectives see below.

Requirements:

The successful candidates should:

- Hold (or be about to earn) a Master's degree (or equivalent) in Physics, Chemistry, Materials Science or Electrical Engineering and have demonstrated an outstanding academic performance.
- Have prior research experience and demonstrated potential and enthusiasm to conduct challenging research towards a PhD.
- Have excellent team-working skills and be motivated to work in a highly interdisciplinary and collaborative environment.
- Have very good oral and written English language skills (German language skills are not mandatory).

Offer:

We offer an exciting research environment with an outstanding research infrastructure, and the participation in an international PhD programme providing for a comprehensive training in technical and professional skills. A fellowship of 1365 EUR per month to cover living expenses in Germany will be offered for a period of three years.

How to apply:

Please visit our website (www.ihrs-nanonet.de) for further information and to access the online application platform (available from 10 January 2015).
Applications sent by e-mail are not accepted.

The application deadline is **20 February 2015**.
Incomplete and post-deadline applications will be disregarded.

The IHRS NANONET is committed to an equal opportunity policy. Admission will be offered to qualified candidates without regard to race, gender, or disability.

Further information: www.ihrs-nanonet.de

Project	**NANONET 2015-1-C1**
Title	**Fabrication of large area and atomically flat MoS_2 nanosheets for electronic devices**
Leading PI	**Prof. Dr. Xinliang Feng**
Leading Institution	TU Dresden, Institute of Macromolecular Chemistry
Collaborations (Involving stay of the student at collaborator)	Dr. Artur Erbe (HZDR), Prof. Dr. Gianaurelio Cuniberti (TUD), Prof. Dr. Gotthard Seifert (TUD)

Summary

Graphene the atomically thinnest two-dimensional (2D) layer of hexagonally arranged network of carbon atoms has laid down the foundation of exciting new science in the area of two dimensional layered materials. After the successful implementation of graphene for various device applications, researchers have now started seeking other 2D atomic crystals, such as, isolated mono and few layers of hexagonal boron nitride (hBN), molybdenum disulphide (MoS_2), and transition metal dichalcogenides (TMDCs). The goal of this research is to develop the effiencet synthesis of thin layer TMDCs using top-down exfoliation (mechanically and liquid assisted) and bottom-up techniques, such as, transition metal sulphurization, thermal decomposition of thiosalts, and vapor transportation.

The successful candidate will carry out:

- Optimization of deposition parameters (substrate pre-treatment, substrate temperature, precursor used, etc) for synthesis of monolayer MoS_2 film using chemical vapour and liquid assisted exfoliation techniques.
- Structural, compositional, optical and morphological investigations of the monolayer MoS_2 film using XRD, HRTEM, XPS, Photoluminescence, Raman spectroscopy and AFM techniques.
- Fabrication of ultrathin transistors and photodetectors using semiconducting MoS_2 monolayer.

We aim at attracting the best talent in the respective research fields and expect the following:

- An outstanding university degree (master or equivalent) in inorganic chemistry, organic chemistry, electrochemistry, materials science or related fields
- Previous experience in organic, polymer or inorganic synthesis
- Experience with thin film deposition processes for soft-materials or fabrication of electronic devices
- Very good interpersonal and communication skills, in particular, the ability to effectively work in collaborative research efforts
- An independent, target- and solution-driven work attitude
- Inter- and multidisciplinary thinking
- Strong motivation and interest to join one of the most ambitious interdisciplinary research clusters
- Fluency in English - written and oral

Project	**NANONET 2015-1-C2**
Title	**Conductive polymer carpets**
Leading PI	**Prof. Dr. Rainer Jordan**
Leading Institution	TU Dresden, Chair of Macromolecular Chemistry
Collaborations (Involving stay of the student at collaborator)	Prof. Dr. Manfred Helm and Dr. Artur Erbe (HZDR), Prof. Dr. Xinliang Feng (TUD), Prof. Dr. Gianaurelio Cuniberti (TUD)

Summary

Aim of the project is the development and characterization of 2D conductive polymer carpets based on graphene for molecular electronics [1-4]. The link between the conjugated polymer and the graphene sheet and the orientation of the polymer will be key aspects of this project as in conventional methods, neither a specific link nor orientation/order can be addressed which strongly impairs overall performance of the nanocomposites. The defined synthesis of conductive polymer carpets will be assessed by advanced characterization methods such as various local probe spectroscopy on the micrometer and nanometer range, scanning probe techniques and full characterization of the electronic properties. First experiments already showed the feasability of our approach. The project is focussing on the chemical aspects of the preparation of the polymer carpets. However, the physico-chemical characterization will be an important aspect of the project and will be performed in close collaboration with research groups within NanoNet and the cluster of excellence in Dresden (cfaed). Furthermore, patterning of the carpets on the micro- and nanometer scale with advanced lithographic techniques in combination with molecular self-assembly will be a crutial and also attractive aspect of the project [5].

The succefull PhD candidate is ideally a chemist or has a solid chemical background and should be familiar with modern techniques of polymer synthesis. The candidate must be able to conduct a project with intensive collaborations with several groups for the detailed physico-chemical characterization of the novel materials.

References

[1] I. Amin, M. Steenackers, N. Zhang, A. Beyer, X. Zhang, T. Pirzer, T. Hugel, R. Jordan, and A. Gölzhäuser, *Polymer Carpets*, Small **6**, 1623-1630 (2010).

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[5] T. Chen, I. Amin, and R. Jordan, *Patterned Polymer Brushes*, *Chem. Soc. Rev.* **41**, 3280-3296 (2012).

Project	**NANONET 2015-1-C3**
Title	**Hybride nano-perovskites**
Leading PI	**Prof. Dr. Brigitte Voit, Dr. Anton Kiriy**
Leading Institution	IPF
Collaborations (Involving stay of the student at collaborator)	Prof. Dr. Stefan Mannsfeld (TUD)

Summary

The past few years have sparked an enormous interest in a new class of semiconductors based on mixed organic–inorganic halide (hybrid) perovskites, e.g., $CH_3NH_3PbX_3$ or $CH_3NH_3SnX_3$ [X= Cl, Br, or I] mainly due to their great appeal for device applications such as photovoltaic cells [1-4]. Although the first efficient solid-state perovskite cells were only reported mid 2012, rapid progress was made with energy conversion efficiencies reaching a confirmed 17.9% by 2014. Moreover, the perovskite structures exhibit ambipolar charge transport with very high electron and hole mobilities that exceed 2000 cm^2/Vs and 300 cm^2/Vs, respectively, and display metal-like conductivity in a doped state [5]. In addition, perovskites possess a number of other attractive properties, such as photoconductivity, photo- and electroluminescence, ferroelectricity and nonlinear optical properties [5]. Solution processability of such materials is another key property which makes them very attractive for device applications such as all solid state solar cells, light-emitting devices, and transistors. So far, these exciting phenomena were explored for perovskites bulk and thick films, but their properties at the nanoscale level are practically unknown.

This multidisciplinary project aims to develop general methods for preparation of high-quality nanostructures of organic–inorganic halide perovskites and to investigate their fundamental physical and chemical properties. 1D-nanoperovskites (nanowires) and ultrathin, few-layer films (2D-nanoperovskites) are the focus of this project. Template-directed methods will be employed to synthesize nanoperovskite hybrids making use of highly oriented pi-conjugated polyelectrolyte molecules as templates. We are particularly interested in the electrical conductivity, charge carrier mobility, photo-/electro-luminescence, excision generation / splitting within these 1D and 2D nanoperovskite nanostructures. We expect that low-dimensional perovskites might display novel properties that originate from quantum-confinement and interfacial effects. Exploring these properties is another major goal of the project.

As the project is strongly multidisciplinary, we seek a PhD student with a relatively broad educational background in material science and chemistry, preferable also with a good understanding of physics.

References

[1] M.M. Lee, J. Teuscher, T. Miyasaka, T.N. Murakami, and H.J. Snaith, *Efficient hybrid solar cells based on meso-superstructured organometal halide perovskites*, Science **338,** 643–647 (2012).

[2] J. Burschka et al., *Sequential deposition as a route to high-performance perovskite-sensitized solar cells*, Nature **499,** 316–319 (2013).

[3] M.A. Green, A.H. Baillie, and H.J. Snaith, *The emergence of perovskite solar cells* Nature Photonics **8**, 506 (2014).

Project	**NANONET 2015-1-E1**
Title	**Bionanosensors technology with integrated nanowire devices**
Leading PI	**Prof. Dr. Gianaurelio Cuniberti**
Leading Institution	TUD, Institute of Materials Science
Collaborations (Involving stay of the student at collaborator)	Dr. Artur Erbe (HZDR, fabrication of the devices), Dr. Walter Weber, Prof. Dr. Thomas Mikolajick (NaMLab, characterization of the devices)

Summary

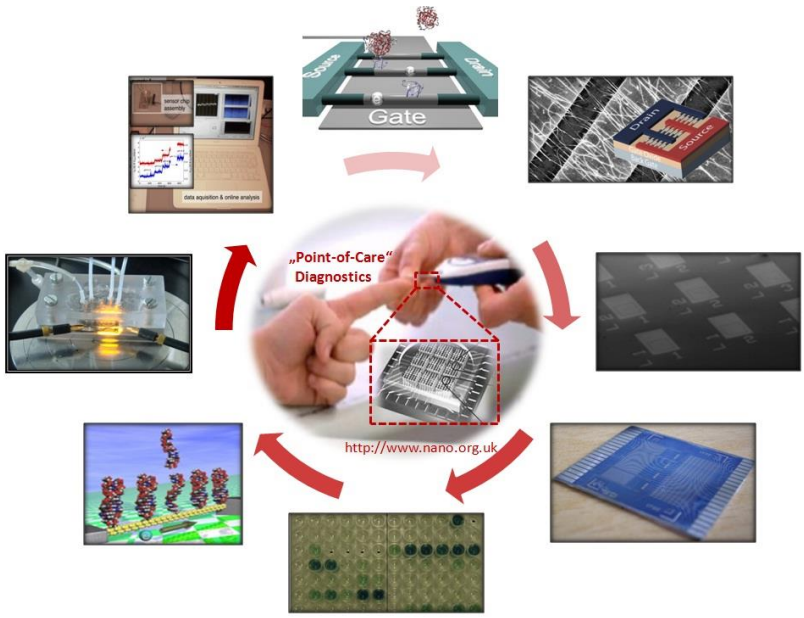
Work will be focused on the investigation of inorganic functional units, functionalization techniques, and the development of nanowires (NW) based bio-electrical sensors with further pushing this development towards point-of-care diagnostics concept.

The targeted objectives of the PhD work are precisely determined as:

(I) Development of biosensor device based on the NW nanoscaled sensors for field effect and impedimetric detection of molecules and single cells, respectively.

(II) Development of the sensor area bio-functionalization schemes to achieve the sensor specificity (e.g. DNA sensing of influenza virus).

(III) Fabrication of microfluidic chips, containing multiple sensor elements, placed in the known locations, for specific disease diagnostics, based on molecular recognition and electrical properties of cells.



The candidate should be highly motivated, interdisciplinary thinking, ready to acquire skills in microfabrication, electrical device characterization, programming, biochemistry. Ability to work in international teams is an important requirement.

Background: Master or an equivalent degree in biotechnology, biology, chemistry, programming skills are advantageous.

Project	**NANONET 2015-1-E2**
Title	**Silicon nanowires under stress**
Leading PI	**Dr. Artur Erbe**
Leading Institution	HZDR
Collaborations (Involving stay of the student at collaborator)	Dr. Jochen Kerbusch (HZDR), Prof. Dr. Sibylle Gemming (HZDR), Prof. Dr. Thomas Mikolajick (NaMLab), Dr. Walter Weber (NaMLab), Dr. Larysa Baraban (TUD)

Summary

The top-down fabrication of silicon nanowires facilitates the integration of these nanostructures into large electronic circuits and allows for the controlled investigation of their properties under various environmental conditions. Based on junctions generated with bottom-up grown nanowires, it has been shown that strain effects in the nanowires have a large influences on the mobility of the charge carriers in the wires and can be used to optimize the devices for ampipolar operation [1]. When deforming the top-down grown nanowires mechanically, the influence of stress on the electronic transport through the nanowires can be investigated. The bending will be accomiplished with nanowires, which are produced on flexible substrates, which are bent using a mechanically controllable break junction setup [2]. This bending leads to a stretching of the silicon wires and thus induces stress inside the wires. We will perform these measurements in ultra-high vacuum, in order to prevent uncontrolled surface modifications, which deteriorate the electrical properties of the wires. Under these conditions, we will also study the temperature dependence of the conductance of the nanowires, which reveals the transport mechanisms inside the nanowires. These studies will therefore contribute to the design of nanowires, which are suitable for the use in integrated electronic nanocircuits.

References

[1] A. Heinzig, T. Mikolajick, J. Trommer, D. Grimm, and W.M. Weber, *Dually Active Silicon Nanowire Transistors and Circuits with Equal Electron and Hole Transport*, Nano Lett. **13,** 4176–4181 (2013).

[2] L.A. Zotti et al., *Revealing the Role of Anchoring Groups in the Electrical Conduction Through Single-Molecule Junctions*, Small **6,** 1529–1535 (2010).

Project	**NANONET 2015-1-P1**
Title	**Simulation of local potentials and magnetic moments at conductive domain walls in multiferroic substrates**
Leading PI	**Prof. Dr. Sibylle Gemming**
Leading Institution	HZDR
Collaborations (Involving stay of the student at collaborator)	Dr. Artur Erbe (HZDR), Dr. Anton Kiriy (IPF), Prof. Dr. Brigitte Voit (IPF), Virtual Institute Memriox (HZDR)

Summary

The thesis focuses on density-functional based modeling of local conductivity changes at the domain boundaries in ferroic materials with the aim to exploit such materials as tunable substrate for organic electronic materials.

Polarization domain walls in ferroelectric materials cause local variations of the electrostatic potential, which can trap charge carriers and thus lead to an enhanced local conductivity along lines on the surface [1]. Such local variations of the surface may also be considered as substrates for the targeted adsorption of molecular components. The possibility to structure such domains optically or by applied external electric fields may be employed to organize monomers for organic electronic films on such a switchable substrate.

For multiferroic materials, previous investigations have shown that also ferromagnetic coupling can arise at such boundaries in materials that are antiferromagnetic otherwise [1,2]. Such couplings have successfully been determined in the material system Y-Mn-O, which is in the focus here [3,4]. Even mobile 2D electron gases have been realized and described theoretically by DFT methods [5].

References

[1] J. Seidel et al., *Conduction at domain walls in oxide multiferroics*, Nature Materials **8**, 229-234 (2009).

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[5] S. Gemming and G. Seifert, *$SrTiO_3(001)|LaAlO_3(001)$ multilayers: A density-functional investigation*, Acta Mater. **54**, 4299-4306 (2006).

Project	**NANONET 2015-1-P2**
Title	**Evolution of the electronic properties of contact materials at the nano-scale**
Leading PI	**Prof. Dr. Sibylle Gemming**
Leading Institution	HZDR
Collaborations (Involving stay of the student at collaborator)	Dr. Artur Erbe (HZDR), Prof. Dr. Jürgen Fassbender (HZDR) Dr. Stefan Facsko (HZDR)

Summary

The thesis aims at the experimental and simulation-based investigation of the electronic structure of contacts and contact materials for nano-electronic devices with particular focus on the deviations from the bulk properties due to the spatial confinement in the contact region. Specifically transition metal chalcogenide nanostructures are in the focus oft he investigations, as joint theoretical and experimental investigations have revealed a fascinating wealth of mechanical and electronic properties in small-scale structures such as clusters, wires, platelets and hollow elements such as tubes, fullerenes, and octahedra.

We could show that preparation of small Mo_mS_n species with a pulsed arc cluster ion source (PACIS) allows control of the overall composition and the specific atom arrangement at the termination sites [1, 2], which is important for contacting and functionalization. Within the thesis this method will be extended by a break junction setup to capture small paticles and determine the electronic properties.

Calculations with the DFTB-method and scanning probe measurements have shown that composition modulations reflect the thermodynamic conditions during the structure formation, which lead to a termination with specific, well-defined and addressable local electronic states [4, 5]. In particular, molybdenum sulphide wires from the sulphur-poor regime exhibit metallic conductance derived from the electronic d states of the metallic core, which is surrounded by insulating chalcogenide atoms [5]; such wires are flexible and undergo a symmetry-induced metal-insulator transition upon torsion [6, 7], which may be exploited for logical or sensing purposes. Calculations for other compositions may accompany the experimental work.

References

[1] S. Gemming, G. Seifert, N. Bertram, T. Fischer, M. Götz, and G. Ganteför, *One-dimensional $(Mo_3S_3)_n$ clusters: Building blocks of clusters materials and ideal nanowires for molecular electronics*, Chem. Phys. Lett. **474**, 127 (2009).

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Project	**NANONET 2015-1-P3**
Title	**Modeling adsorption and transport properties of molecular wires grown by on-surface polymerization**
Leading PI	**Prof. Dr. Gianaurelio Cuniberti, Dr. Francesca Moresco**
Leading Institution	TU Dresden, Institute for Materials Science
Collaborations (Involving stay of the student at collaborator)	Prof. Dr. Sibylle Gemming (HZDR), Prof. Dr. Brigitte Voit (IPF), Prof. Dr. Xinliang Feng (TUD)

Summary

Conjugated polymer chains (1D structures) can be grown on-surface under ultra-high vacuum (UHV) conditions in a controlled way. Recently, long molecular wires and graphene nanoribbons have been demonstrated [1,2].
In NanoNet, experimental work is ongoing in collaboration with the groups of B. Voit and A. Kiriy (IPF Dresden) to control the on-surface polymerization process, investigating several possible reaction mechanisms.
The present project aims to theoretically investigate the properties of the molecular wires, which are growth on-surface and investigated by STM in the Moresco group (TU Dresden).
Ab-initio theoretical studies will be performed on the adsorption and electronic properties of the molecular wires on metal surfaces. Using DFT based molecular dynamics simulations we will investigate on-surface chemical reactions of polymerization and the effects of hybridization between electronic states in the wires and metal substrate ("metallization"). Besides, calculation and analysis of STM images and STM spectroscopy will be performed.

References

[1] J. Cai et al., *Atomically precise bottom-up fabrication of graphene nanoribbons*, Nature **466**, 470 (2010).

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