TNT 2017
Trends in NanoTechnology

Dresden (Germany)
June 05-09, 2017

Abstracts & Posters Book

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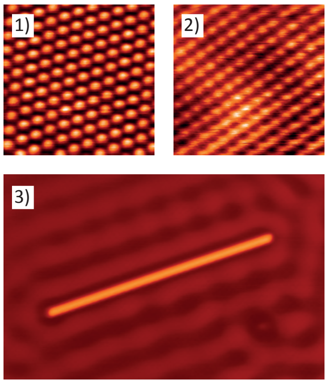

Fig. 1: STM measurement on Ag(111) at T = 9.8 K with running CC-cooler (5 x 5 nm)
Fig. 2: nc-AFM QPlus measurement on NaCl(100) (3 x 3 nm)
Fig. 3: Ag nanowire on Ag(111) surface (40 x 30 nm)

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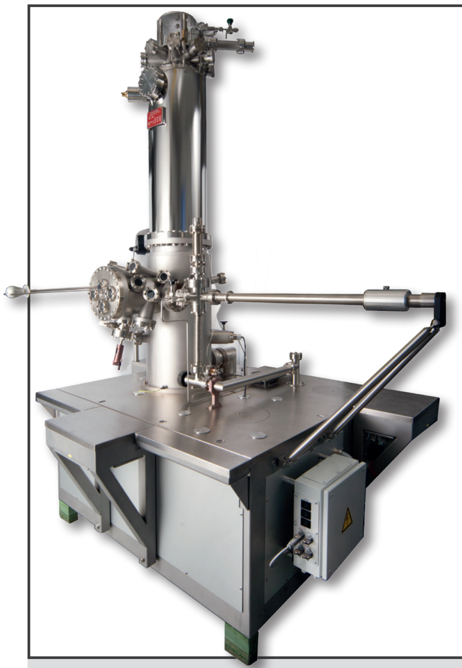

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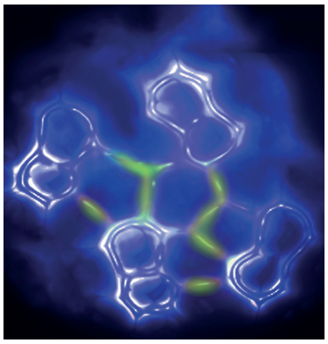

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8-hydroxyquiline molecular assemblies on Cu(111).
Xiaohui Qiu et al. (China)

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TNT2017 index

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On behalf of the International and Technical Committees, we take great pleasure in welcoming you to Dresden (Germany) for the 18th "Trends in NanoTechnology" International Conference (TNT2017).

TNT2017 is being held in large part due to the overwhelming success of earlier TNT Nanotechnology Conferences.

This high-level scientific meeting series aims to present a broad range of current research in Nanoscience and Nanotechnology worldwide, as well as initiatives such as MANA/NIMS, Adolphe Merkle Institute, IBEC, ICN2 or cfaed. TNT events have demonstrated that they are particularly effective in transmitting information and promoting interaction and new contacts among workers in this field. Furthermore, this event offers visitors, exhibitors and sponsors an ideal opportunity to interact with each other.

This year, a Graphene one-day Symposium will again be organized within TNT2017 in collaboration with ICN2 (Spain) and cfaed (Germany).

One of the main objectives of the Trends in Nanotechnology Conference is to provide a platform where young researchers can present their latest work and also interact with high-level scientists. For this purpose, the Organizing Committee provides every year travel grants for students. In addition, awards will also be given to young PhD students for their contributions presented at TNT. Grants and awards are funded by the TNT Organization in collaboration with private bodies and several governmental/research institutions.

TNT is now one of the premier European conferences devoted to nanoscale science and technology.

We are indebted to the following Scientific Institutions, Companies and Government Agencies for their financial support: Phantoms Foundation, C'Nano GSO, Scienta Omicron and FEI.

We would also like to thank the following companies and institutions for their participation: CSInstruments, Springer Nature, Raith, SURAGUS GmbH, Physical Electronics GmbH, Scienta Omicron, cfaed - TU Dresden and HORIBA Scientific.

In addition, thanks must be given to the staff of all the organizing institutions whose hard work has helped planning this conference.

TNT2017 Organising Committee

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The Cluster of Excellence 'Center for Advancing Electronics Dresden' (cfaed) of Technische Universität Dresden comprises eleven research institutes in Saxony. Further members are the Technische Universität Chemnitz, two Max Planck Institutes, two Fraunhofer Institutes, two Leibniz Institutes and the Helmholtz-Research Center Dresden-Rossendorf. About 300 scientists are working in nine research paths to investigate completely new technologies for electronic information processing. These technologies are inspired by innovative materials such as silicon nanowires, carbon nanotubes or polymers or based on completely new conceptions such as circuit fabrication methods by self-assembling structures, e.g. DNA-Origami. The orchestration of these new devices into heterogeneous information processing systems with focus on their resilience and energy-efficiency is also part of cfaed's research program. To complement the Cluster, the Collaborative Research Center (CRC) 912 'Highly Adaptive Energy-Efficient Computing' (HAEC) has been integrated in cfaed. Both, cfaed and HAEC, are coordinated by Prof. Dr.-Ing. Dr. h.c. Gerhard Fettweis, who holds the Vodafone Chair Mobile Communications Systems at TU Dresden.

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Monday – June 05, 2017

14:00-15:00	REGISTRATION	
15:00-15:15	**TNT2017 Opening Ceremony - Welcome and Introduction**	
15:15-15:45	**Luis Hueso** (CIC nanoGUNE, Spain) Spin transport, spinterface and spin photovoltaics in molecular films	K
15:45-16:00	**Manoko Maubane** (University of the Witwatersrand, South Africa) From Carbon Shells to Multipods - The role of nickel particle shape and size	O
16:00-16:15	**Petra Pötschke** (Leibniz-Institut für Polymerforschung Dresden e.V. , Germany) Polymer-SWCNT composites for recovering waste heat into electrical energy	O
16:15-16:45	**Mikhael Bechelany** (IEMM-CNRS, France) Engineering of Interfaces for Preparing new Functional Materials	K
16:45-17:30	**Coffee Break**	
17:30-18:00	**Xiaodong Zhuang** (Dresden University of Technology, Germany) 2D Materials for supercapacitors	I
18:00-18:15	**Ye Liu** (Dresden University of Technology, Germany) Doped Single-Walled Carbon Nanotubes for Flexible Thermoelectric Applications	O
18:15-18:30	**Xiaoyu Han** (University College London, UK) A Targeted Functional Design for Highly Efficient and Stable Cathodes for Rechargeable Li-Ion Batteries	O
18:30-18:45	**Lifeng Liu** (International Iberian Nanotechnology Laboratory, Portugal) Monolithic Cobalt Phosphide Nanowire Electrodes for Efficient and Durable Water Splitting	O
18:45-19:00	**Siddik Icli** (Ege University, Turkey) Photosynthesis; Miracle of Organic Life and its Technologies	O

Tuesday – June 06, 2017

GRAPHENE DAY

09:00-09:30	**Claudia Backes** (Universität Heidelberg, Germany) Liquid-exfoliated transition metal dichalcogenides: from spectroscopic metrics to functionalisation	K
09:30-10:00	**Ute Kaiser** (Ulm University, Germany) Properties of two-dimensional materials by high-resolution low-voltage aberration-corrected TEM	K
10:00-10:30	**Andrey Turchanin** (Friedrich Schiller University Jena, Germany) Carbon-based van der Waals heterostructures of 2D materials	K
10:30-11:00	**Coffee Break - Poster Session - Instrument Exhibition**	
11:00-11:30	**Xinliang Feng** (Technische Universitaet Dresden, Germany) Graphene and Organic 2D Materials: Grand Challenges and Opportunities	K
11:30-12:00	**Francesco Bonaccorso** (IIT-Graphene Labs / BeDimensional, Italy) The science and technology of graphene and inorganic 2D crystals	K
12:00-12:30	**Vladimir Falko** (National Graphene Institute, UK) Electronic and optical properties of 2D atomic InSe crystals	K
12:30-13:00	**Thomas Heine** (Universität Leipzig, Germany) Two-dimensional crystals containing phosphorus	K
13:00-14:30	**Lunch** (Not included)	
14:30-18:00	**PARALLEL SESSION GRAPHENE TRACK A** **PARALLEL SESSION GRAPHENE TRACK B**	

K: Keynote / I: Invited / O: Oral

Tuesday – June 06, 2017

PARALLEL SESSION - GRAPHENE TRACK A

14:30-15:00	**Marc Chaigneau** (HORIBA Scientific, France) Tip Enhanced Optical Spectroscopy of 2D materials – from graphene to TMDCs	I
15:00-15:15	**Stephan Adam** (SURAGUS GmbH, Germany) Challenges and Insights by Electrical Characterization of Large Area Graphene Layers	O
15:15-15:30	**Christophe Adessi** (Université Claude Bernard Lyon I, France) First principle investigation on thermoelectric properties of transition metal dichalcogenides: Beyond rigid band model	O
15:30-15:45	**Alexei Nazarov** (Lashkaryov Institute of Semiconductor Physics NASU, Ukraine) Electrical Conductivity and micro-Raman Sectroscopy of Graphene Layer Deposited on SiO$_2$ Dielectric and Subjected to Electron Beam Irradiation	O
15:45-16:00	**Michele Pisarra** (Universidad Autónoma de Madrid, Spain) Graphene on SiO$_2$ under ultrahigh pressure	O
16:00-16:30	**Coffee Break - Poster Session - Instrument Exhibition**	
16:30-17:00	**Paolo Bondavalli** (Thales Research & Technology, France) Graphene based supercapacitors : results perspectives and potential industrial implementation	I
17:00-17:15	**Pedro Costa** (King Abdullah University of Science and Technology, Saudi Arabia) Rational Design of Graphene-Based Materials for Supercapacitors	O
17:15-17:30	**Jian Zhang** (cfaed TU Dresden, Germany) Efficient Hydrogen Production by Tailoring Electrocatalysts with Fast Water Dissociation Kinetics	O
17:30-17:45	**Moumita Kotal** (Korea Advanced Institute of Science and Technology, Korea) Nitrogen and Sulfur Co-doped Holey Graphene Aerogel For High-performance Compression-Tolerant All Solid-State Supercapacitors	O

PARALLEL SESSION - GRAPHENE TRACK B

14:30-15:00	**Julio Gomez** (Universidad Autónoma de Madrid, Spain) Isolation of Highly Stable Antimonene under Ambient Conditions. Optical and Electrical Properties	K
15:00-15:30	**Siegfried Eigler** (Freie Universität Berlin, Germany) Controlled Chemistry of Oxo-functionalized graphene and graphene oxide	K
15:30-16:00	**Armin Gölzhäuser** (Bielefeld University, Germany) Carbon Nanomembranes (CNM): 2D Materials Beyond Graphene	K
16:00-16:30	**Coffee Break - Poster Session - Instrument Exhibition**	
16:30-17:00	**Zhenxing Wang** (AMO GmbH, Germany) Graphene-based high-frequency electronics	I
17:00-17:15	**Renhao Dong** (TU Dresden, Germany) Interfacial Synthesis of 2D Polymers and 2D Supramolecular Polymers	O
17:15-17:30	**Emre Gür** (Atatürk University, Turkey) Magnetron Sputtered WS$_2$ Thin Films	O
17:30-17:45	**Jian Xiang Lian** (UMONS, Belgium) Ordered Non-Covalent Functionalization of Graphene by Controlled Formation of 2D Supramolecular Self-Assemblies at the Graphene Surface Forming Hybrid vdW Heterostructures	O
17:45-18:00	**Dmitry Kvashnin** (National University of Science and Technology MISiS, Russia) One-atom-thick 2D material based on CuO. Experimental observations and theoretical study	O

K: Keynote / I: Invited / O: Oral

Wednesday – June 07, 2017

09:00-09:30	**Stefania D'Agostino** (IIT, Italy) New Trends in Computational Plasmonics	K
09:30-10:00	**Xavier Bouju** (CEMES / CNRS, France) Gold monolayer islands on a polar AlN(0001) surface	K
10:00-10:30	**Dmitry A. Ryndyk** (University of Bremen, Germany) Atomistic nanoscale device modeling: charge and heat transport in large-scale systems	I
10:30-11:15	**Uzi Landman** (Georgia Tech, USA) Small is Different: Old Questions - New Paradigms	K
11:15-11:45	**Coffee Break - Poster Session - Instrument Exhibition**	
11:45-13:00	**Poster Session**	
13:00-14:30	**Cocktail Lunch (offered by TNT2017 organisers)**	
14:30-15:00	**Christian Joachim** (CEMES/CNRS, France) One-way rotation of a single molecule-rotor	K
15:00-15:30	**Anne-Sophie Duwez** (University of Liege, Belgium) Probing single molecules with AFM: Force, motion, dynamics, and function	K
15:30-16:00	**Francesca Moresco** (TU Dresden, Germany) Mechanics with single molecules: Manipulation with the STM tip	K
16:00-17:00	**Coffee Break - Poster Session - Instrument Exhibition**	
17:00-17:30	**Markus Maier** (Scienta Omicron, Germany) Electrical Transport Measurements with Atomically Precise Probes	I
17:30-18:00	**Takashi Uchihashi** (MANA-NIMS, Japan) Switchable supramolecular motors with surface chirality	K
18:00-18:30	**We-Hyo Soe** (CEMES/CNRS, France) Controllable single molecule gear	K
18:30-19:00	**Danny Porath** (The Hebrew University of Jerusalem, Israel) Novel DNA-Based Molecules and Their Charge Transport Properties	K

19:30	**Conference Dinner**

K: Keynote / I: Invited / O: Oral

Thursday – June 08, 2017

11:30-11:45	**Adriana Szeghalmi** (Friedrich Schiller University, Germany) Tailored nanoporous SiO_2 thin films for antireflection coatingst	O
11:45-12:00	**Eva Schubert** (University of Nebraska-Lincoln, USA) Hybrid Materials from Sculptured Thin Films and Applications	O
12:00-12:30	**Georg Johannes Schmidt** (Martin-Luther-Universität Halle-Wittenberg, Germany) Nanopatterned complex oxides - key to new physics	K
12:30-13:00	**Philippe Leclère** (University of Mons - UMONS, Belgium) About the Quantitative Mapping of the Mechanical Properties of Polymeric Materials at the Nanoscale	K
13:00-14:30	**Lunch** (Not included)	
14:30-15:00	**Lucia Delogu** (University of Sassari, Italy) New hight troughput technologies reveal the impact of nanomaterials with human primary immune cells	K
15:00-15:15	**Maria Emmeleia Gianneli** (Attana AB, Sweden) Towards prediction of in vivo behavior of nanoparticles: A QCM platform for characterization of nanoparticle - cell interactions in a complex biological milieu	O
15:15-15:30	**Nermin Seda Kehr** (WWU-Münster, Germany) Bifunctional Porous Nanomaterials for Cell-Biomaterial Interaction Studies	O
15:30-16:00	**Benjamin Friedrich** (Max-Planck Institute, Germany) Navigation at the micro-scale: Swimming, steering,synchronization of biological microswimmers	K
16:00-16:30	**Coffee Break - Poster Session - Instrument Exhibition**	
16:30-16:45	**Larysa Baraban** (Dresden University of Technology, Germany) Compact nanowire sensors probe emulsion droplets	O
16:45-17:00	**Bergoi Ibarlucea** (TU Dresden, Germany) Ebola biosensing with a gate controlled memristor mode	O
17:00-17:15	**Nadia Licciardello** (Technische Universität Dresden, Germany) Ultrasmall nanoparticles for bioapplications: potential in droplets based microfluidics	O
17:15-17:30	**Jorge Romero-Garcia** (Centro de Investigacion en Quimica Aplicada, Mexico) Biomimetic Synthesis of Polyaniline Catalyzed by Hematine Supported on Graphitic Carbon Nitride	O
17:30-17:45	**Cornelia Palivan** (University of Basel, Switzerland) Design of artificial organelles by combining proteins with synthetic nanocompartments	O
17:45-18:00	**Olga Dement´eva** (Frumkin Inst. of Physical Chem. and Electrochemistry of RAS, Russia) Novel Drug-Templated Mesoporous Silica Nanocontainers and Protocells Based Thereon	O

K: Keynote / I: Invited / O: Oral

Friday – June 09, 2017

PARALLEL SESSION (PhD Student Track A)

09:00-09:15	**Bushra Ali** (Dundalk Institute of Technology, Ireland) Layer-By-Layer multilayer assembly of Graphene oxide with Keggin-type Polyoxometalates for electrocatalysis of Chloroform	O
09:15-09:30	**Andrzej Chalupniak** (ICN2, Spain) Toward integrated detection and graphene-based removal of contaminants in a lab-on-a-chip platform	O
09:30-09:45	**Muhammad Ilyas** (Brunel University London, UK) Structural Analysis of Plasma Exfoliated Graphene Nanoplatelets (GNPs) for the Development of Nano-Cementitious Composites	O
09:45-10:00	**Sandeep Kumar Jain** (Utrecht University, The Netherlands) Graphene mechanics: defects, buckling and domain growth	O
10:00-10:15	**Silvan Kretschmer** (Helmholtz-Zentrum Dresden-Rossendorf, Germany) The mystery of semiconductor to metal phase transition in MoS$_2$ under electron beam	O
10:15-10:30	**Narek Margaryan** (National Polytechnic University of Armenia, Armenia) The Study of Physical Properties of Self-Assembled Graphene	O
10:30-11:30	**Coffee Break**	
11:30-11:45	**Leonardo Medrano Sandonas** (Dresden University of Technology, Germany) Phononics in two-dimensional materials	O
11:45-12:00	**Arevik Musheghyan Avetisyan** (Universitat de Barcelona, Spain) Direct low temperature growth of vertically oriented graphene nanowalls on multiple substrates by Low Temperature Plasma-Enhanced Chemical Vapor Deposition	O
12:00-12:15	**Jae Hoon Yang** (Daegu Gyeongbuk Institute of Science and Technology, Korea) Geometrically Enhanced Asymmetric I-V Characteristics in Graphene Tunneling Diode	O
12:15-12:30	**Sheng Yang** (Technische Universitaet Dresden, Germany) Electrochemical Exfoliation of Layered Conductive Materials	O

PARALLEL SESSION (PhD Student Track B)

09:00-09:15	**Yuki Nakata** (Tohoku University, Japan) Discovery of 2D Mott insulating phase in 1T-NbSe$_2$ atomic layer	O
09:15-09:30	**Martin Hartmann** (University of Technology, Germany) Performance enhancement of carbon nanotube FETs via polymer-based doping control	O
09:30-09:45	**Stephanie Klinghammer** (Technische Universitaet Dresden, Germany) Multiplexed sensing of steroids with silicon nanowire field effect transistors	O
09:45-10:00	**João Albuquerque** (REQUIMTE/UCIBIO/FFUP, Portugal) Bypassing the rumen using lipid nanoparticles	O
10:00-10:15	**Fernando Jiménez** (IMDEA Nanociencia, Spain) Innovative Patterning Method for Modifying few-layer Mos$_2$ Device Geometries	O
10:15-10:30	**Mark-Robert Kalus** (University of Duisburg-Essen, Germany) Ligand-free nanoparticles made by scalable laser synthesis for catalysis applications	O
10:30-11:30	**Coffee Break**	
11:30-11:45	**Seunguk Kim** (Daegu Gyeongbuk Institute of Science and Technology, Korea) Optimizing geometric factors of nano-hole arrays for Label-free bio-detection	O
11:45-12:00	**Jens Natterodt** (Adolphe Merkle Institute, Univ. of Fribourg, Switzerland) Polymer Nanocomposites with Cellulose Nanocrystals made by Coprecipitation	O
12:00-12:15	**Eunhye Baek** (Technische Universitaet Dresden, Germany) Multiplexed Synaptic Modulation and Memory in Ionic Film-coated Si Nanowire Transistors	O
12:15-12:30	**Álvaro Díaz Fernández** (Universidad Complutense de Madrid, Spain) Tailoring Fermi's velocity in topological insulators by an electric field	O
12:30-14:00	**Lunch** (Not included)	

K: Keynote / I: Invited / O: Oral

Friday – June 09, 2017

PLENARY SESSION

14:00-14:15	**Daniel E. Bürgler** (Forschungszentrum Jülich, Germany) Intramolecular variation of spin-polarization within single molecule-surface hybrid	O
14:15-14:30	**Martyna Pingot** (Lodz University of Technology, Poland) New cross-linking method of halogenated butyl rubber nanocomposites	O
14:30-14:45	**Lars Rebohle** (Helmholtz-Zentrum Dresden-Rossendorf, Germany) Millisecond annealing for the nanoscale	O
14:45-15:00	**Zikhona Tetana** (University of the Witwatersrand, South Africa) Nitrogen and Boron doping Effects in Carbon Nanospheres	O
15:00-15:15	**Kumud Malika Tripathi** (Gachon University, Korea) Multifunctional Water Soluble Carbon Nano Onions from Flaxseed Oil for Visible Light Induced Photocatalytic Applications and Label Free Detection of Al(III) Ions	O
15:15-15:30	**Hender Lopez** (University College Dublin, Ireland) Using single nanoparticle tracking to simultaneosly characterize nanoparticle size distribution and nanoparticle-surface interactions	O
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The Chair of Materials Science & Nanotechnology

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TNT2017 Keynotes / Invited contributions

Liquid-exfoliated transition metal dichalcogenides: from spectroscopic metrics to Functionalisation

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Liquid exfoliation has become an important production technique to give access to large quantities of two-dimensional nanosheets in colloidal dispersion.[1] Importantly, this is a highly versatile technique that can be applied to numerous layered materials beyond graphene. These can be cast into films and composites and have proven useful in a number of application areas. However, as produced dispersions contain a nanosheets of various sizes and thicknesses making post-exfoliation size selection extremely important to tap the full potential in the future. We have previously developed a universal and efficient size selection technique termed liquid cascade centrifugation[2] which allowed us to produce monolayer-rich dispersions with monolayer volume fractions up to 75%. Optimisation was made possible because we have realised that nanosheet size and thickness, as well as monolayer content can be quantitatively extracted from optical spectra due to edge and confinement effects greatly facilitating and accelerating the characterisation.[2,3]

We now use this basic understanding and these improvements in sample quality to systematically investigate the effect of the chemical environment on the optical properties of the liquid-exfoliated nanosheets. For example, we show that the A-exciton energy depends on the layer number in a similar way for a number of different TMDs. Furthermore, dielectric screening from additives and solvents can be tracked via this A-exciton layer number dependence making this an ideal fingerprint for noncovalent functionalisation. Last but not least, we show that the ability to dramatically increase the surface area of the layered materials on exfoliation can be used to explore new chemistry and to controllably functionalise either basal plane[4,5] or edge sites (Figure 1).

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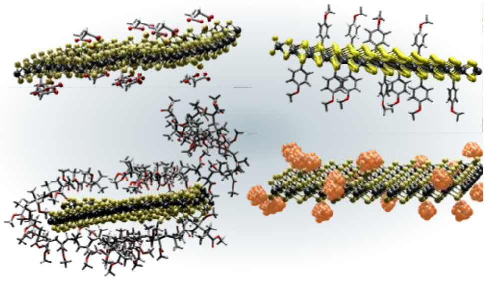

Figure 1. Schematics of functionalized transition metal dichalcogenides via various strategies

Engineering of Interfaces for Preparing new Functional Materials

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Nanostructure science and technology are a broad and interdisciplinary area of research and development that has been exponentially growing in the past few years. Engineered nanomaterials are resources designed at the molecular (nanometer) scale to take advantage of their small size and novel properties which are generally not seen in their conventional bulk counterparts. The two main reasons why nanomaterials can have different properties are: (i) the increase of relative surface area and (ii) the quantum confinement effects leading to novel optical, electrical and magnetic behaviors. In order to apply these nanomaterials in different fields and to increase the throughput of nanostructured materials and devices for energy, environmental and health applications, an efficient engineering of the nanomaterials interfaces is needed.

Here, we used different synthesis techniques such as atomic layer deposition (ALD),[1] electrospinning, electrodeposition, anodisation, nanospheres lithography, 3D printing and the exfoliation of Graphene and BN like Graphene etc. as the main tools for the creation of controlled nanostructured materials and interfaces [2] in which the geometry can be tuned accurately and the dependence of the physical-chemical properties on the geometric parameters can be studied systematically in order to investigate their performances in energy, environmental and health applications. We will show examples of how these methods can be used to create (bio)- fuel cells, [3] single nanopores for sensing and sequencing, [4] membrane for gas purification, osmotic energy harvesting and water treatment, optical sensors and biosensors [5], and bionanocomposites materials for packaging [6], drug delivery [7] and tissue engineering in which the performance varies with the nanostructures/interfaces.

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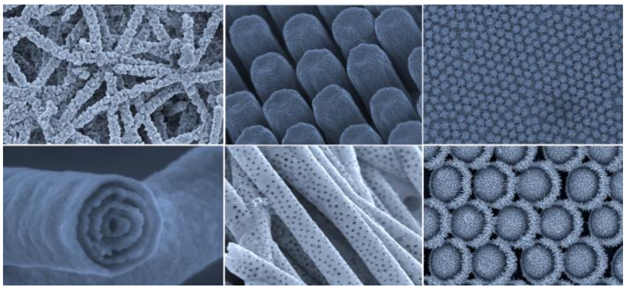

Figure 1. Design of bionanostructures materials for energy, environmental and health applications

The science and technology of graphene and inorganic 2D crystals

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New materials and processes[1] can improve the performance of existing devices or enable new ones,[1-5] with the added values with respect to the current technology to be environmentally benign. In this context, graphene and other inorganic 2D crystals are emerging as promising materials,[1-5] with the opportunity to enable new products/devices.[1] However, a fundamental requirement for the application of 2D crystals in areas such as flexible electronics and energy storage and conversion relies on the development of industrially scalable, reliable, inexpensive production processes.[2] Moreover, the synthesis strategies should provide a balance between ease of fabrication and final material quality with on-demand properties.

Solution-processing[2,6] offers a simple and cost-effective pathway to fabricate various 2D crystal-based (opto)electronic and energy devices, presenting huge integration flexibility compared to conventional methods. Here, I will present an overview of graphene and other 2D crystals for flexible and printed (opto)electronic and energy applications, starting from solution processing of the raw bulk materials,[2] the fabrication of large area electrodes[3] and their integration in the final devices.[7-15]

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Graphene based supercapacitors : results perspectives and potential industrial implementation

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This contribution we will deal with the results recently obtained on supercapacitors with electrodes fabricated using mixtures of graphene based nanomaterials with carbon nanofibers and nanotubes [1]. The electrode fabrication has been performed using a new dynamic spray-gun based deposition process set-up at Thales Research and Technology (patented) [2]. This technique constitute a real breakthrough compared to the classical filtration method because electrodes can be deposited over large areas in a completely automated way, using different kinds of substrates and with a thickness between some nm and up to hundredth of µms [3]. During the presentation we will show the industrial implementation and value chain that has been identified to achieve real industrial devices.

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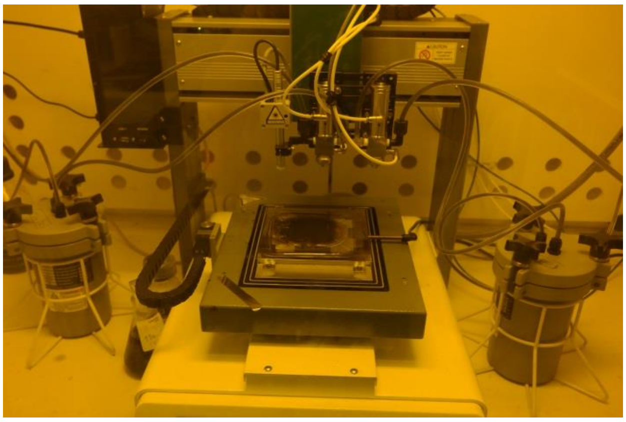

Figure 1. Spray gun deposition machine with two nozzles for nanostructuration.

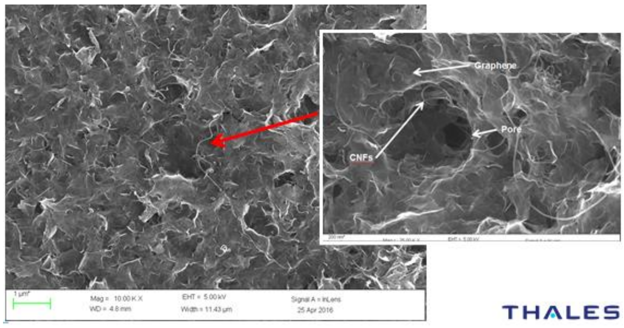

Figure 2. Graphene layer nanostructuration exploiting mixture of graphene and carbon nanofibers

Gold monolayer islands on a polar AlN(0001) surface

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High-power electronic devices require materials with large electron mobilities and densities and large band gaps. Group-III nitride semiconductors are ideal candidates for these applications. Among these materials, aluminium nitride (AlN) has the largest band gap (6.2 eV). It also has unique properties such as small density, large stiffness, large piezoelectric constant, large fracture resistivity, and chemical inertness.

The growth of metallic nanoclusters on insulating substrates and the study of their physical properties are a wide research domain, pushed by the desire to tailor some specific electronic, magnetic, optical and chemical properties for applications. Most metals grow in the form of three-dimensional (3D) clusters at the early stages of their deposition on such substrates. This situation generally results from the unfavourable surface and interface free energies balance involved in the formation of two-dimensional (2D) islands.

We recently elaborate and characterize AlN(0001) thick films, whose surface is polar. We identified the mechanism of charge compensation for one of its (2×2) reconstructions [1]. Here, we show how the deposition of gold atoms on the (2×2)-N_{ad} AlN surface results to the formation of nano-islands.

Noncontact atomic force microscopy images show that gold grows on the (2×2)-N_{ad} reconstructed polar (0001) surface of AlN insulating films, in the form of large monolayer metallic islands. High-resolution images and in-situ reflection high-energy electron diffraction spectra reveal two moiré patterns from which an atomic model can be built. Density functional theory (DFT) calculations confirm this model and give insight into the mechanisms that lead to the stabilization of the monolayer (Fig.1). Gold adsorption is accompanied, first, by a global vertical charge transfer from the AlN substrate that fulfils the electrostatic stability criterion for a polar surface, and second, by lateral charge transfers that are driven by the local chemical properties of the (2×2)-N_{ad} reconstruction. These results open the way to new strategies using polar surfaces to grow metallic monolayers on insulating substrates.

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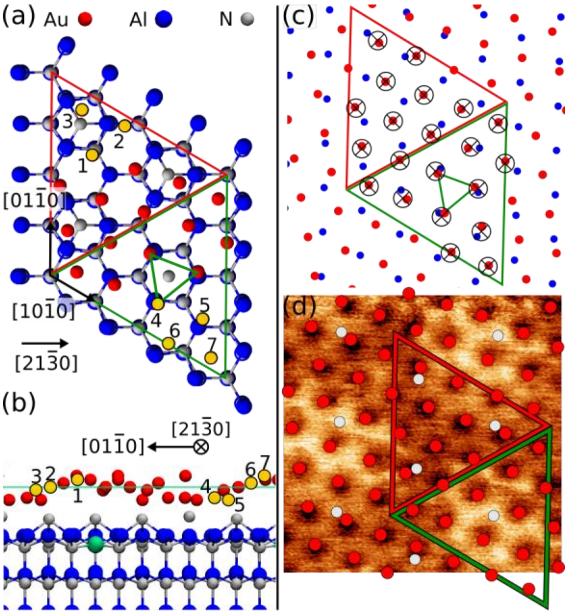

Figure 1. (a) Top view of the DFT optimized structure. (b) Projection along the [2 1 -3 0] axis helps to visualize the different heights of gold atoms with respect to the mean Au plane. (d) NC-AFM image of the Au monolayer on the AlN surface with the superimposed Au atoms calculated positions.

Tip Enhanced Optical Spectroscopy of 2D materials – from graphene to TMDCs

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Raman spectroscopy has become a leading technique in graphene and 2D materials research. It is widely used to determine the number and orientation of layers, the quality of the materials, the presence of defects and their density, and the effects of strain or doping elements. Tip Enhanced Raman Scattering (TERS) is today a mature technique that gives access to all those mentioned information down to the nanoscale, thus providing important insights into he structure of such 2D materials.

In this talk, we'll report results of TEOS (Tip Enhanced Optical Spectroscopy, including TERS and TEPL, Tip Enhanced Photoluminescence) characterization of graphene, functionalized graphene oxide and 2D semiconductors (MoS_2, WS_2 and WSe_2).

We will report on how TEOS characterization can reveal very localized spectra change correlated with the number of layers, the local position of the Fermi level, and breaks of translation symmetry.
We will discuss the impact of TEOS characterization in the studies of single-layer and few layer 2D materials and emphasize the capability of seeing deep-subdiffraction-limited details that can be today correlated with complementary Kelvin probe microscopy and photo-current techniques.

Figures

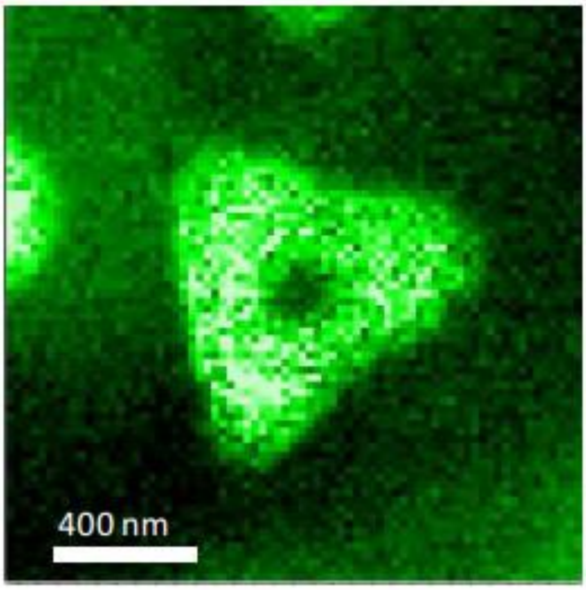

Figure 1. TERS/TEPL image – MoS_2 flake on Si

New Trends in Computational Plasmonics

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Plasmonics has seen an incredible boost during the past few decades as a promising route for nanophotonic devices. Metallic elements act as optical antennas and can strongly enhance the efficiency of several photophysical phenomena.
The resonant coupling between light and metallic (or heavily doped semiconductor) nanostructures enables the possibility to squeeze the electromagnetic fields in sub-wavelength volumes, greatly enhancing optical absorption and scattering phenomena. Electrodynamics methods have been proven to be useful and powerful tools to theoretically investigate and optimize plasmonic systems with respect to their macroscopic interactions with absorbers or emitters placed in their proximities[1]. Anyway, with the help of new fabrication techniques it is nowadays possible to realize very narrow junctions or nanogap features between larger metallic elements, so that control of light-matter interactions can be achieved at the sub-nanometer scale. This requires to adopt new theoretical schemes able to overcome the limits of the classical vision and to go towards "quantum".

Recent experimental studies have demonstrated in fact, that quantum mechanical effects, such as electron spill-out and tunneling as well as nonlocal screening, cannot be neglected as distances between metallic elements approach the subnanometer length-scale[2]. Such quantum mechanical effects have thus operated a revolution in plasmonics, stimulating a number of theoretical and experimental studies aiming to describe the atomistic structure of matter. In this talk, an overview on the last developments in computational plasmonics, highlighting their limits and potentialities, is given with the idea to stress the trends and identify the challenges in the field. Several efforts have already been done to include quantum effects in the calculation of the optical properties of nanoparticles by introducing non-local corrections to the classical dielectric constant[3] or by recurring to the *Jellium-Model* based TD-DFT (*Time Dependent Density Functional Theory*) approach[4]. However, such calculations neglect the atomistic nature of matter and as a consequence they do not success in describing experimental results, highlighting the need for better models to take into account the quantum behavior of electrons. Standard TD-DFT seems to be, thus, the most suitable approach for a complete quantum mechanical treatment of nano-plasmonic systems but it becomes computationally unaffordable for particle sizes of the order of several hundreds or thousands of atoms. To this regards, *Density Functional-based Tight-Binding Approximation*, together with its Time-Dependent (DFTB) derivation, seems to be a promising frontier of computational plasmonics[5]. DFTB is based on the second order expansion of the Kohn-Sham energy functional around a reference density of neutral atomic species and it can be proved to be an efficient scheme for describing the optics of plasmonic systems under particular conditions. With an appropriate choice of the Slater-Koster parametrization, results that are in good agreement with Ab Initio calculations can be achieved at a much reduced computational cost. This opens the avenues towards a new era of plasmonics and, in particular, molecular plasmonics.

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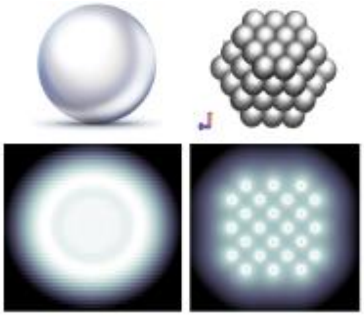

Figure 1. Jellium model (left) and fully-atomistic (right) groundstate electron density for a NP within DFT.

New hight troughput technologies reveal the impact of nanomaterials with human primary immune cells

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Abstract

Nanotechnology nowadays is expanding its legacy in medicine by implementing approaches aimed to delivering therapeutics and developing new diagnostic and imaging tools [1]. However, before any translational application of nanotechnology in medicine, a critical step is represented by the assessment of their impact on the complexity of the immune system [2]. In this context, is mandatory to study the immunological impact of some of the main promising nanomaterials for biomedical applications such as carbon nanotubes (CNTs), graphene, lipid nanocapsules (NCs) and super paramagnetic iron oxide nanoparticles (SPIONs) on the different immune cell populations. Recently we focused our attention on these new nanomaterials in order to clarify their potential to be applied in therapy and diagnostic applications, taking also advantage from their intrinsic immunomodulayory properties. One example of this approach is here reported for graphene, particularly on its oxidized form (GO). We investigated the effects of several types of thoroughly characterized GO sheets, different in their lateral dimension and functionalization, on human primary lymphomonocytes from healthy donors. Wide range of assays looking at cell viability, cell activation, and molecular interaction were done. Moreover, to better dissect the immunological effects of these nanomaterials on individual cells, we applied single-cell mass cytometry to evaluate the effect of functionalized GOs on 15 cellular populations corresponding to 200 nodes of distinct but logically interconnected cell sub-populations. We than used whole-transcriptomic analysis (Illumina BeadArray) for functional and molecular characterization of GOs on human T-cells and monocytes. Notably, only the functionalized GO ($GONH_2$) was able to induce a specific dendritic cell and monocyte activation skewed toward a Th1/M1 response, as demonstrated by the increased production of classic M1 cytokines (TNFα, IL6, and CCL4) [**Fig.1**]; inducing also the overexpression of pathways critical for the development of an effective anti-tumor immune response (i.e. interferon signaling) [**Fig.2**]. A positive impact of nanomaterials on the immune system, able to trigger both immune suppression or immune activation, is a new concept helpful in the development of new nanoscale platforms in medicine. These new platforms, indeed can be investigated as immunotherapy tools, vaccine carriers, adjuvants, and drug delivery systems to target pathology or inflammatory and inflammation-associated disorders.

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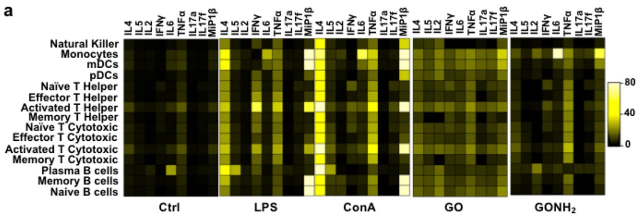

Figure 1. **Analysis of the immune cell behavior using CyTOF2**

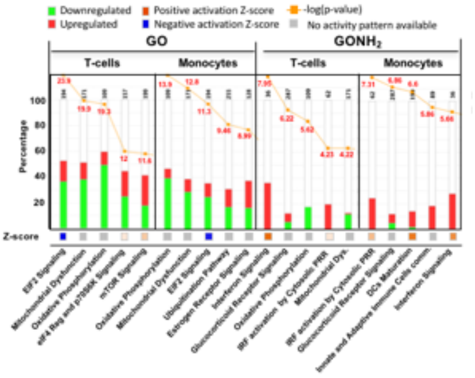

Figure 2. **Gene expression impact of GO and $GONH_2$ on T- and monocyte cell lines**

Probing single molecules with AFM: Force, motion, dynamics, and function

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In 1952, Erwin Schrödinger wrote that we would never experiment with just one electron, one atom, or one molecule.[1] Forty years later, methods derived from scanning probe microscopies allowed us to manipulate single atoms and molecules, and even single bonds.[2] Single molecule force spectroscopy, which consists in trapping and stretching a molecule between an AFM tip and a surface, enables to probe (and/or to induce) molecular processes in situ and in real time through the application of mechanical forces. Such elegant experiments have provided unprecedented insights into the structure and function of many (biological) systems.[3]

Force, dynamics, and function can now be probed at the single-molecule level, but this exploration of single entities is only in its infancy. Physicists are eager to know whether the phenomena observed at this scale obey the laws we know for ensemble of species or will force us to rethink our understanding of physics. Chemists can now play with single bonds, orient molecules and trigger a chemical reaction between single entities. Biologists and biophysicists are now able to investigate molecular-level processes involved in living organisms, such as muscle contraction, cell locomotion and division, or transport processes. Much of the exquisite and detailed information about how biomolecular machines operate has been gleaned from direct measurements made on single molecules.

Here, we will discuss some of our recent results in the field of AFM-based single molecule force spectroscopy on bio-inspired systems, like the investigation of how small binders perturb the dissociation mechanisms of DNA, single atom exchange in supramolecular polymers, the measurement of the force generated by a synthetic molecular machine and the real time capture of folding/unfolding transitions in synthetic foldamers.[4]

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Controlled Chemistry of Oxo-functionalized graphene and graphene oxide

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The structure of graphene oxide is a matter of discussion since more than 150 years. Many aspects of the chemical structure of graphene oxide is known nowadays. Ideally, the hexagonal lattice of graphene carries oxo-addends. We introduced that material, termed as oxo-functional graphene (oxo-G). Oxo-G is a novel class of materials, which bears a hexagonal carbon lattice, a high surface purity and on-plane functional groups in majority. HRTEM micrographs demonstrate the lattice structure.[1] Moreover oxo-G bears no relevant amounts of oxidative debris and thus, graphene oxide can be considered as a one-component system.[2]. Oxo-G can be used to control the chemistry of surface functional groups and we identified endoperoxides as source of the toxicity of oxo-G. Toxic endoperoxides can be removed to allow bio-applications.[3] Controlling the on-plane chemistry of oxo-G gives access to controlled structures and with a defined composite we demonstrate the extension of the life-time of perovskite/PCBM solar cells.[4] Rationally designed graphene derivatives have the potential to boost the performance in applications, such as information storage or solar cells.

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Electronic and optical properties of 2D atomic InSe crystals

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We present the analysis of electronic band structure of InSe and (other III-VI semiconductors) films, from the stoichiometric mono-layer to N-layer films, and we describe the resulting optical properties of these 2D materials [1,2]. This study is based on the ab initio DFT and related multi-orbital tight-binding model analysis of the electronic band structure and wave functions in the two-dimensional N-layer InSe crystals, and it is compared to the results of luminescence spectroscopy of this material. We show [1-3] that the band gap in InSe (and GaSe) strongly depend on the number of layers, with the variation from 2.7 eV (3.3 eV) in the monolayers to 1.25eV (2 eV) in crystals with N>10. We find that the conduction-band-edge electron mass in few-layer InSe is quite light (comparable to Si), which suggests opportunities for high-mobility devices and the development of nanocircuits. In contrast, the valence band in mono-, bi- and trilayer InSe is flat, opening possibilities for strongly correlated hole gases in p-doped systems

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Graphene and Organic 2D Materials: Grand Challenges and Opportunities

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The discovery of graphene one decade ago has inspired the development of other two-dimensional (2D) materials with periodic network structure and topographical thickness of atomic/molecular level. They have emerged as the new paradigm of materials with enormous potentials, ranging from electronics and optoelectronics to energy technology, membrane, sensing and biomedical applications. However, to transform the fundamental studies of graphene and 2D materials into practical applications, many critical challenges have to be solved. The future research and application of these materials urgently call for the efficient and reliable chemical synthesis and processing, which have to play a key enabling role.

In this lecture, our recent efforts on the top-down exfoliation of graphite and bottom-up synthesis of structurally well-defined graphene will be presented. The solution exfoliation of graphite is relying on the smart processing of graphitic precursors at the few-layer thickness level under the electrochemical control. This strategy offers the reliable means to produce high quality, solution-processable graphene on a large scale and at low cost. To introduce a defined bandgap into graphene materials, a bottom-up synthetic strategy is demonstrated, providing structurally defined nanographenes and graphene nanoribbons with tailor-made properties at the atomic level. Towards the synthesis of emerging organic 2D materials, we will present our recent developments on the 2D conducting/conjugated polymers and supramolecular polymers with structural control at the atomic/molecular-level as well as at the meso-scale. The rational processing and assembly of graphene and 2D materials provide the access to novel hierarchical structures and hybrid systems with different complexities. As the result, we will present some prominent applications with using graphene and organic 2D materials as well as their hybrids across the fields of electronics, fuel cells, supercapacitors and micro-supercapacitors as well as batteries.

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Navigation at the micro-scale: Swimming, steering, synchronization of biological micro-swimmers

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Single biological cells can swim in a liquid, harnessing mechanical forces generated by ten-thousands of nano-scale motor proteins. Their swimming is controlled by chemical and mechanical signals for directed navigation. A prime example is represented by swimming sperm cells, which are guided by concentration gradients of signaling molecules towards the egg. Here, I review a unique navigation strategy along helical paths employed by sperm cells of external fertilizers, which is remarkably robust in the presence of sensing noise [1]. In a second part, I will present a biological example of "embodiment control" in a biological microswimmer, where interaction with the physical environment results in a coordinated swimming gait by a mechanical self-stabilization mechanism [2]. Ultimately, navigation principle invented by nature can be exploited for the design of intelligent artificial microswimmers.

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Figures

Figure 1. Artistic representation of "The Computational Sperm Cell", navigating in response to chemical cues toward the egg.

Carbon Nanomembranes (CNM) : 2D Materials Beyond Graphene

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Carbon Nanomembranes (CNMs) are extremely thin (~1nm), synthetic two-dimensional (2D) layers or sheets with tailored physical, chemical or biological function [1]. Their fabrication scheme utilizes a sequence of molecular monolayer assembly on a solid surface and radiation induced cross-linking in two dimensions. The cross-linked monolayer is then released from the surface, forming a self-supporting nanomembrane with properties that are determined by properties of the monolayer. Depending on the desired applications, CNMs can be engineered with a controlled thickness, elasticity and surface functionalization. Helium ion microscopy, spectroscopic methods and functional tests are applied to investigate the structure and composition as well as permeation properties. Helium Ion Lithography is used the fabrication of well-defined nanopores [2] and perforated CNMs are tested as ballistic membranes for the separation of gases and liquids.

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Isolation of Highly Stable Antimonene under Ambient Conditions. Optical and Electrical Properties

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Graphene paved the way for the rising of a whole family of 2D materials. Graphene is a semimetal with zero-gap and transition metal dichalcogenides present a band gap in the range 1.5-2.5 eV [1], inappropriate for some optoelectronics applications where 0.1-1.5 eV are preferred. Few-layer black phosphorous (BP) [2] presents an energy gap within this range. However, it is highly hygroscopic [3]. In the same group in the periodic table we also find antimony, a silvery lustrous, non-hygroscopic element with a layered structure similar to that of BP. Theoretical calculations [4] point towards a band gap suitable for these optoelectronics applications. We report micromechanical and liquid-phase exfoliation of antimony down to the single-layer regime and experimental evidence of its high stability in ambient conditions [5, 6]. We also present optimized optical identification [7] and preliminary results on the conductive properties of few-layer antimonene, which point to be governed by topologically protected surface states. In this context, Probe-Assisted Nanowire (PAN) lithography is introduced; a novel technique to create nanoelectrodes that has allowed probing the electrical properties of tiny few-layer antimonene flakes.

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Figures

Figure 1. Atomic force microscopy image of an antimonene flake representing its stability in ambient conditions.

Two-dimensional crystals containing phosphorus

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Abstract

Phosphorene, a single layer of black phosphorus, has been discovered in 2014 and, despite its low chemical stability, has been considered as promising material for two-dimensional electronics as it has a band gap and high charge carrier mobilities. However, the air-instability of phosphorene strongly limits its application in research, development and potential applications, and thus alterative materials inhibiting similar properties, i.e. high carrier mobility and small band gap, are welcome new members in the family of two-dimensional materials.

We will introduce two new two-dimensional crystals that contain phosphorus. Germanium phosphide, GeP_3 (Figure 1), is a metallic layered material with arsenic-type puckered honeycomb structure that has been experimentally reported in 1970. We show that its single and double layers are low band gap semiconductors, while it becomes metallic for 3 layers and more. Its small band gap, high absorption coefficient and high mobility makes it a promising material for electronic and optoelectronic applications.

We will discuss other isostructural and isoelectronic compounds of the layered materials composed of Group 14/15 elements.

Another interesting layered phosphorus containing material is PdPX, with X=S, Se, Te (Figure 2). Also here, the layered material is known from experiment. The monolayer has electronic properties that appear to be ideal for photocatalytic water splitting with band edges matching the potentials of hydrogen and oxygen evolution reactions. The Pd centres are expected to have beneficial catalytic activity, in particular at the edges of PdPX nanoparticles.

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Figures

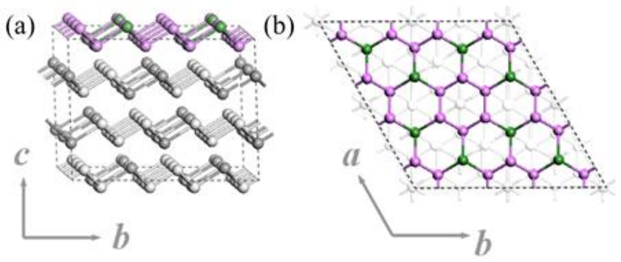

Figure 1. Structure of bulk GeP_3 in a 2×2×1 supercell from side (a) and top (b) views. Pink and green balls represent P and Ge atoms, respectively.

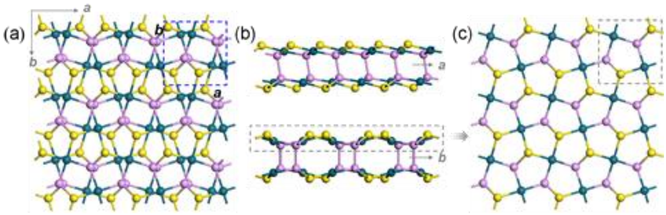

Figure 2. Atomic structure of PdPX ML from top (a) and side (b) views and (c) the sublayer isolated from a ML (unitcell is enclosed by the dashed blue or grey line).

Spin transport, spinterface and spin photovoltaics in molecular films

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Spin injection and transport into molecular semiconductors has attracted great interest recently, especially due to the small sources of spin decoherence in these materials [1]. However, there are still many open questions in this nascent field which range from the actual spin polarization at metal/molecular interfaces to the integration of molecular functionalities into spintronic devices.

In this talk I will review several experimental highlights from our group.

By using bathocuproine (BCP) and fluorinated copper phthalocyanine (FCuPc) we have unambiguously proved that spin transport occurs via molecular levels, finally dismissing any eventual role of metallic filaments or defects in the electronic transport [2,3]. Our experiments point to the critical role of the interfacial barriers for carrier injection into the molecular levels. Moreover, in the FCuPc case we have shown concomitant spin transport and photoresponse. Thanks to the emergence of two molecular-based properties, four distinguishable resistance states adjustable by light and/or magnetic field can be configured in a simple 2-bit memory cell [3]. Further recent results in this wide topic, merging spin transport with the photovoltaic effect of C_{60} fullerenes will be shown [4].

I also will present spin valves based on rare-earth quinolines. Here we highlight the role of metal/molecular hybridization in the spin polarization and its possible control [5-7].

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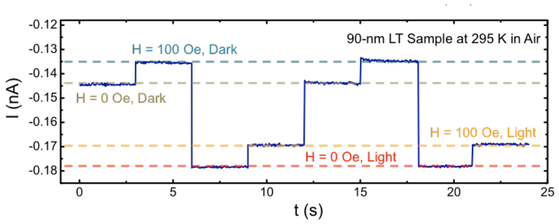

Figure 1. Demonstration of four distinctive resistance states reachable by operation of the magnetic field and the light irradiation in a FCuPc-based organic spin valve. Extracted from reference [3]

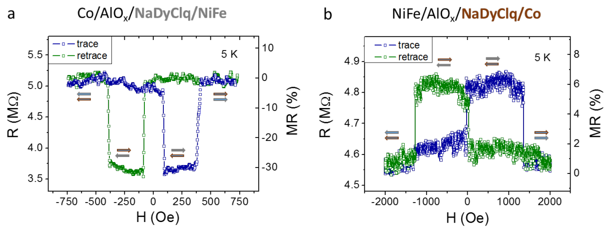

Figure 2. Inversion of the spin polarization (detected as magnetoresistance), due to the different hybridization between molecular NaDyClq and NiFe or Co ferromagnetic metals. Extracted from reference [7]

One-way rotation of a single molecule-rotor

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Passing through a molecule-motor, the tunneling current shot noise can drive the one-way rotation of its rotor [1,2,3]. Here the local quantum access to the vibronic modes of its first excited states is delivering minute energy to this rotor using the very local tunneling inelastic effect induced by the STM tip with a precision better that 10 pm [4,5]. We demonstrate that a ratchet-like ground state rotation potential energy curve is not necessary for the rotation to occur and anyway the micro-reversibility principle forbid the existence of such a ground state [6]. We will show that a relative shift in energy between the maxima of this ground state and the minima of the employed excited states is necessary to reach a unidirectional rotation. The rotor speed of rotation and its rotation direction are both controlled by this shift [6], pointing out the necessity of a careful design of both the ground and excited states of the next generation of molecule-motors to be able to generate a motive power at the atomic scale.

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Properties of two-dimensional materials by high-resolution low-voltage aberration-corrected TEM

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To obtain structural and electronic properties of two-dimensional electron-beam-sensitive materials by analytical low-voltage spherical and chromatic aberration-corrected transmission electron microscopy we developed further three main topics:

(1) Theory and image processing [1-3]: For exact calculation of high-resolution (HR)-TEM images for low-Z materials at low voltages, the contribution of inelastic scattering cannot be neglected. For calculation of low-voltage energy-filtered (EF)-TEM images, the contributions of elastic and inelastic scattering to the image intensity cannot be separated from each other because the inelastic scattering amplitudes are influenced by elastic scattering, and vice versa. Moreover, we study the dependence of the signal-to-noise ratio, atom contrast and resolution on electron dose and sampling in order to achieve highest resolution.

(2) Sample preparation [4,5]: We demonstrate our successful method to clean graphene as a prerequisite for its use in TEM. Sandwiching radiation-sensitive low-dimensional objects in-between two graphene layers allows an effective reduction of electron-beam-induced damage of the objects. Moreover the exchange of hydrogen by deuterium allows to image the object at a factor of two higher electron dose.

(3) Low-voltage Cc/Cs-corrected TEM instrument [6,7]: We show unprecedented high resolution at low voltages from 80kV down to 20kV using our brand-new spherical and chromatic aberration corrected *SALVE* microscope [8]. We show that lowering the energy of the imaging electrons down to 20kV increases contrast and prevents various e.g. molecules on graphene from electron-beam stimulated damage.

The application of our strategies [9-11] on deriving the properties of different two-dimensional crystalline (ion-implanted graphene, MoS_2, $MoSe_2$, $TaSe_2$, WS_2, SiO_2) and amorphous (monolayer carbon, SiO_2) materials will be demonstrated.[12]

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About the Quantitative Mapping of the Mechanical Properties of Polymeric Materials at the Nanoscale

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Dynamic Atomic Force Microscopes (AFM) are often used to probe nanomechanical properties of soft materials, in particular for polymers. The last two decades have seen numerous efforts to interpret height and phase images in terms of mechanical properties and dissipating processes. Beyond the technical difficulties, mostly related to a proper knowledge of the size and shape of the tip, extracting quantitative information requires a model (ideally providing analytical expressions), in turn allowing the recorded data to be analyzed. Any attempt to model oscillation behavior when the tip touches the sample faces several difficulties, making models of the interaction truly cumbersome.

On one hand, when the tip is in contact with the sample, it is possible to get quantitative mapping of the mechanical parameters by a technique named *Contact Resonance AFM*. On the other hand, with the recent development of *multifrequency AFM* based techniques, analysis of the cantilever motion in dynamic AFM can describe the force acting on the tip, from which we can hopefully intuit the viscoelastic properties the studied surface. Progress in the field of instrument/cantilever calibration, and methods of force measurements set the stage for a critical examination of the different physical models commonly used in this growing field of research. These models are of paramount importance for our understanding and interpretation of the data to provide the (ideally quantitative) mapping of the material mechanical properties. In this work, we will review most of them by illustrating their capabilities but also their limitations on a series of samples based on polymer blends and block copolymers.

Material property mapping based on this approach faces many problems, mainly since the measurements are performed too rapidly, provoking the appearance of viscous forces. More importantly, when the sample is very soft, the tip penetrates the surface and its interaction with the surface may include entropic forces, capillary forces arising from surface curvature that is not usually considered. Actually, many of the methods developed so far employ a linear approximation, treating the mechanical response as changing the parameters of an effective cantilever resonance assumed in rigid contact with the surface.

By using *Intermodulation AFM* data [1-2], we clearly show that we can go beyond the linear response and the rigid interaction models to explain the AFM data. Our analysis based on the dynamic force quadratures, very like the macroscopic *Dynamic Mechanical Analysis*, clearly show that significant viscous response may be explained by a soft material flow, giving the surface its own dynamics. From the comparison with simulations of the dynamics of the system including the surface deformation in a simple model describing the cantilever eigenmode coupled to a linear viscoelastic surface, we can find remarkably good agreement between experiment and simulation, providing quantitative mapping of the mechanical properties of (very soft) polymeric-based materials essentially at any point of the (viscous) surface.

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Electrical Transport Measurements with Atomically Precise Probes

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A major challenge in the development of novel devices in nano- and molecular electronics is their interconnection with larger scaled electrical circuits. Local electrical probing by multiple probes with precision on the atomic scale can significantly improve efficiency in analyzing electrical properties of individual structures on the nano-scale without the need of a full electrical integration.

The LT NANOPROBE is a sophisticated instrument that merges the requirements of a 4-probe system, efficiently and precisely navigated by a scanning electron microscope (SEM) and at the same time satisfies the needs for high performance SPM. The excellent stability in the pm range allows for atomic resolution in STM and nc-AFM (QPlus) and expands applications from electrical probing on the nanometer scale towards tunneling and force spectroscopy and the creation of atomically precise structures. The system is operated near thermal equilibrium and temperatures below 5K, specifically also during simultaneous SEM imaging and navigation. The system has been developed towards an extremely low thermal drift in the range of 100pm/h, which is the most important ingredient to allow for enough measurement time on extremely small structures.

We will present measurements that prove the performance level of the instrument, specifically the low thermal drift and stability as well as QPlus AFM measurements, which become important if nanostructures are deposited on an insulating substrate for a better electrical decoupling. We will also show the newest technology improvements, such as high frequency capabilities and optical access for pumped probe experiment. Future technology challenges as well as applications and scientific drivers for this type of scientific instrumentation will be discussed.

Figures

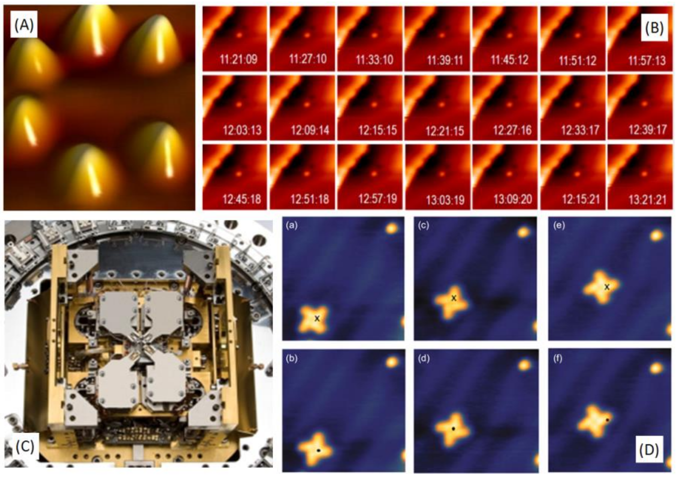

Figure 1. a)STM atom manipulation on Au(111) @ T<5K. Data Courtesy by Ch. Joachim et al., PicoLab, CNRS, France b)Drift measurements STM on Au(111) @ T<5K. Image size 20 nm^2, Ugap = 0.5 V, IT = 0.5 nA. Total measurement time of approx. 2hrs, resulting in a lateral drift < 1.3Å/h. c)Picture of the LT NANOPROBE stage, showing thermal shields, spring suspension, and 4 dedicated shared stack SPM scanners. d)STM manipulation of acetylbiphenyl (ABP) molecules on the Au(111) surface @ T<5K. Data Courtesy by F. Eisenhut et.al. ; Eur. Phys. J. Appl. Phys. (2016) 76.

Mechanics with single molecules: Manipulation with the STM tip

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Mechanical molecular systems can provide an alternative route to transmit information at the nanoscale and could compete in terms of high-clock frequency and robustness to radiations with electronic, optical and magnetic devices. STM at low temperature is a powerful tool to study mechanics at the nanoscale, because it combines on-surface chemistry to synthetize complex molecules in an ultraclean environment, molecular assembly to form ordered complex nanostructures, and atomic-scale manipulation to study conformational changes and mechanical properties of single molecules.

In this talk, recent results will be reviewed, where single molecules and molecular nanostructures are formed on surface and manipulated by tunneling electrons on metallic and semiconducting surfaces. The transmission of motion between molecules will be discussed, towards the construction of molecule-machines.

In particular, hydrogen-bonded supramolecular nanostructures can be precisely moved on a gold surface by voltage pulses applied through the STM tip [1]. Such nanostructures can generate work by moving the load of a single atom [2].

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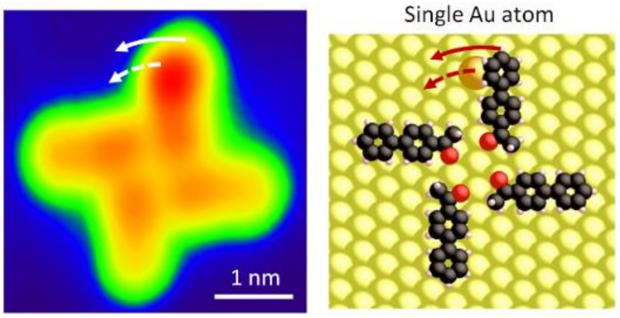

Figure 1. A supramolecular nanostructure composed of four 4-acetylbiphenyl molecules and self-assembled on Au (111) was loaded with single Au adatoms and studied by STM. By applying voltage pulses to the supramolecular structure, the loaded Au atoms can be rotated and translated in a controlled manner.

Novel DNA-Based Molecules and Their Charge Transport Properties

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The DNA double-strand recognition, as well as the ability to manipulate its structure open a multitude of ways to make it useful for molecular electronics. Step by step we improve the synthesized constructs and the measurement methods of single DNA-based molecules. I will present new DNA-based metalized molecules and report on our measurements of their energy level structure and transport properties. I will also report new measurements on dsDNA molecules that point out to an unexpected mechanism.

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Figures

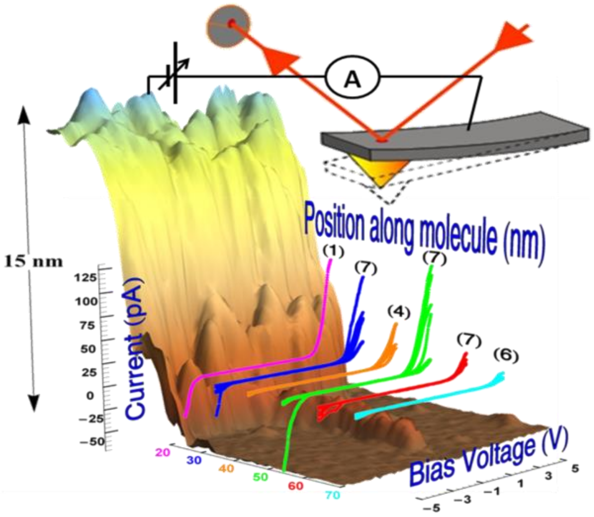

Figure 1. Three dimensional presentation of a G4-DNA molecule protruding from under a sharp metal border. The AFM tip and electrical circuit are illustrated. On top of the molecule appear current-voltage curves measured on ten different molecules.

Atomistic nanoscale device modeling: charge and heat transport in large-scale systems

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First, I will briefly overview the standard approach for charge transport at nanoscale, based on the Density Functional Theory and single-particle Green Function method for coherent Landauer transport. Being about 15 years old and realized in the number of available atomistic codes, the standard approach is very successful in describing the coherent transport at nanoscale in low-dimensional and molecular materials and devices, also with complex geometries, many-terminal configurations and nonequilibrium states at finite voltages. However, extension of the theoretical and computational methods to more complex, large-scale, and interacting systems is still a challenge. I will present our recent results concerning the extended contacts [1]. We apply this approach to find a contact resistance of side CNT-metal contacts, transfer length in graphene-metal contacts and electronic properties of the diodes with CNT channel and asymmetric contacts (with the electrodes made of different metals). The other important developments are phonon transport and thermoelectric phenomena [2], and dephasing [3]. Finally, we discuss the realization of new quantum transport methods at nanoscale [4] in the DFTB+ code [5].

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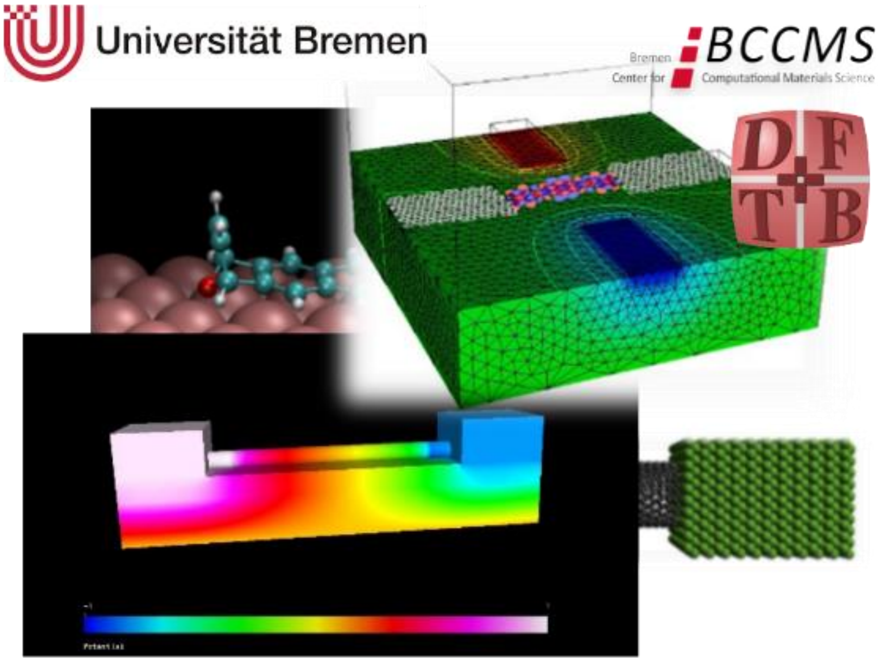

Nanopatterned Complex Oxides – Key to New Physics

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Complex oxides are promising materials for future electronic applications, especially because of the large variety of properties. They can be ferromagnetic, ferroelectric, conducting, insulating, piezoelectric and much more. In order to use them for future nanoelectronics it is necessary to develop suitable patterning processes. For many of these materials the latter is quite a challenge because they are much more stable to standard dry etching techniques than for example II/VI, III/V, or group IV semiconductors and unlike most metals they may lose or change their relevant properties if patterned by simple physical patterning techniques. A good example is insulating $SrTiO_3$ which is often used as a substrate and by most dry etching techniques is turned conducting. Because of this lack of suitable nanopatterning techniques the investigation of interesting physics is often limited to macroscopic structures.

One of our main research topics concerns the development of reliable nanopatterning processes for various oxides. The applications are widespread and range from the tuning of magnetic properties in ferromagnetic $La_{0.7}Sr_{0.3}MnO_3$ by shape anisotropy[1] in large areas of nanostructures to the investigation of magnetotransport in nanostructures patterned from the well known electron gas in $LaAlO_3/SrTiO_3$ heterostructures[2]. In the latter for example we have observed a resistance anomaly which is undetectable in large area structures and which points out that the low temperature transport in this material system is entirely based on filaments which appear at structural domain walls in the substrate while the larger part of the interface is completely insulating[3].

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Figures

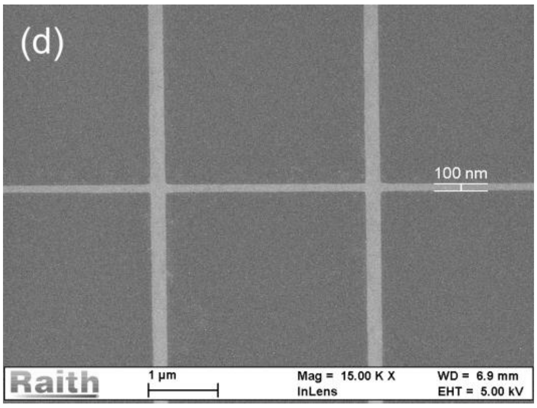

Figure 1. Nano-Hall bar patterned from $LaAlO_3/SrTiO_3$

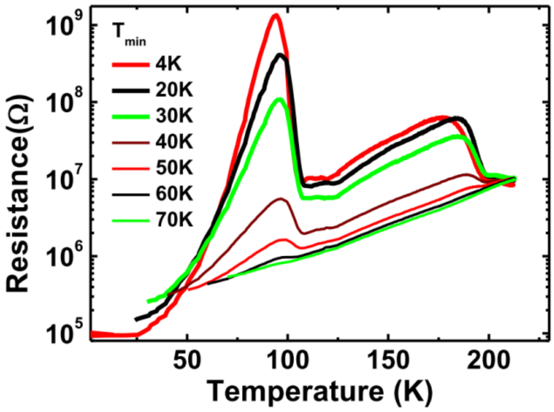

Figure 2. Resistance of an LAO/STO nanostructure measured during warm-up from low temperature. For the different curves the minimum temperature is varied.

Controllable single molecule gear

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An experimental demonstration is presented of the fundamental component of a planar single-molecule mechanical machinery: a molecule gear intentionally assembled on a Au(111) surface. A Scanning Tunneling Microscope (STM) is used as the sole tool to build, controllably manipulate and observe the molecule gear step by step rotation[1]. A hexa-*t*-butyl-pyrimidopentaphenyl- benzene ($C_{64}N_2H_{76}$; HB-NBP) molecule 1.3 nm in diameter was mounted and centered on one atomic scale axis on Au(111). Our investigation shows that the combination of molecule design, molecule manipulation protocol and surface atomic structure selection leads the functioning of the molecule gear. The rotation of this molecule gear is done step-by-step and totally under control, demonstrating nine stable stations in both rotational directions. Each station can be identified comparing calculated and experimental images. For each calculated image, the stable position of the gear was obtained using molecular mechanics calculations.

To bridge between the above molecule gear and solid state nanogears and to transmit the motion from (and to) the nanoscale to the mesoscale for possible applications like data input on an atomic scale circuit or information encoding, we present also the e-beam naofabrication of solid-state SiO_2 nanogears with diameters ranging from 350 nm to down to a 40 nm[2]. Those gears can be manipulated using an Atomic Force Microscope (AFM) tip on a polycrystalline gold surface, to construct a train of gears where mechanical motion can be transmitted from one to another by mastering the surface friction. In conclusion, we will discuss possible ways to bridge the remaining gap between the solid state 40 nm and the molecule 1.3 nm in diameter nanogears (or between a 15 nm thick solid state gear and a molecule gear 0.6 nm in height).

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Figures

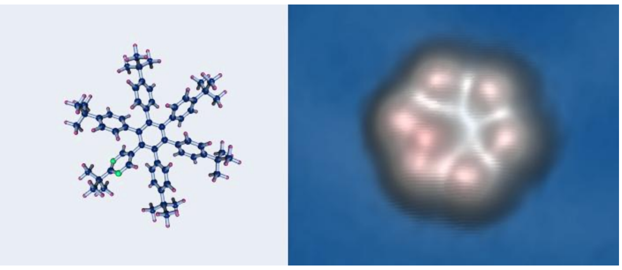

Figure 1. single gear molecule; ball-and-stick model (left) and LT-STM image (right).

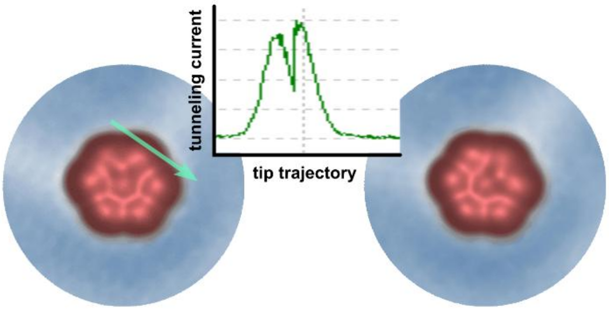

Figure 2. Controllable gear rotation from one station to another induced by a tip apex molecule manipulation. The molecule gear is mounted on the herringbone kink of Au(111) reconstructed surface. The rotation mechanics was followed by recording the tunneling current during the one step molecule gear rotation.

Carbon-based van der Waals heterostructures of 2D materials

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By stacking various atomically thin sheets (e.g., graphene, MoS_2, or BN), novel van der Waals (vdW) heterostructures can be engineered even if these material combinations cannot be grown directly by physical vapor deposition techniques. In this way, vdW heterostructures with tailored electronic and optoelectronic properties can be generated by combining metallic, insulating and semiconducting nanosheets. Here, the fabrication and characterization of all-carbon vdW heterostructures consisting of graphene, carbon nanomembranes (CNMs) and organic semiconductor nanosheets will be presented.[1-6] It will be shown how other carbon-based low dimensional materials (e.g., fullerenes, dyes, or metalorganic catalysts) can be integrated into these layered structures enabling for new functionallity.[3-4] Moreover, implementation of the assembled hybrid all-carbon vdW heterostructures will be demonstrated in (i) high performance field-effect devices[2,6]; (ii) electrochemical nanosensors; (iii) photo-switchable transistors.

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Switchable supramolecular motors with surface chirality

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Surface-supported molecular motors are nanomechanical devices of particular interest in terms of future nanoscale applications [1-3] However, the molecular motors realized so far consist of covalently-bonded groups that cannot be reconfigured without undergoing a chemical reaction. Here we demonstrate that a supramolecule can be used to realize a rotary molecular motor capable of *in-situ* directional switching through variation of surface chirality [4]. A platinum-porphyrin-based supramolecularly-assembled dimer was fabricated by sublimation of the molecules onto Au(111) in vacuum. It was found that dimer species were trapped preferentially at an atomic defect in the herringbone structure. The dimer could be rotated with high directionality by exciting only the molecule-motor part of the dimer using the tunneling current of STM. The ''axle'' of the molecular-rotor moiety of this dimer is defined by the atomic defect and the center of the molecule, which in this case is the Pt atom of the metalloporphyrin. Rotational direction of the molecule-motor is determined solely by the surface chirality of the dimer. Notably, the chirality and hence the rotational direction can be inverted, through a process involving an intra-dimer rearrangement, by selecting an appropriate applied bias voltage. In view of biological motors made of supramolecules, our finding promises construction of complex molecular machineries resembling biological systems at a smaller scale and on a solid surface.

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Figures

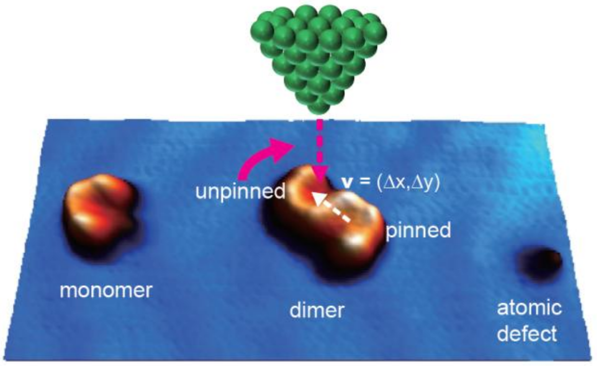

Figure 1. Three-dimensional presentation of an STM image of a Pt-MTBPP dimer molecule taken at 5 K. A monomer and an atomic defect are also visible nearby. Tunneling current injection from STM tip at the center of the unpinned molecule is schematically illustrated.

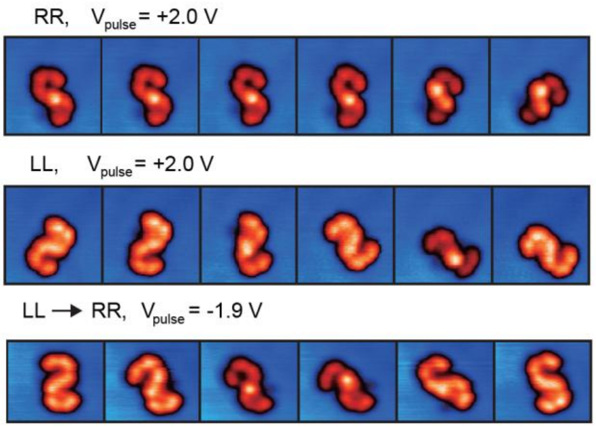

Figure 2. (top) Series of STM images of a dimer undertaking directional rotations at V_{pulse} = +2.0 V. The chirality of the dimer is RR. (middle) Series of STM images of a dimer with a chirality of LL. (bottom) Series of STM images of a dimer undergoing chirality change induced at V_{pulse} = -1.9 V.

2D Materials for Supercapacitors

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Triggered by discovery of graphene, more and more two-dimensional (2D) nanomaterials have been developed by versatile methods. The supercapacitor performance of these new 2D materials have caught wide interests for both science and industry communities. In this presentation, we will show the progress from our group.

Smart micro-/nano-devices or stimuli-responsive devices, which can be engineered to respond to a variety of inputs, such as pH, ions, heat, light, magnetic field, etc., have also attracted substantial attention due to a wide range of needs for smart modern electronics. However, it is still a great challenge to integrate various kinds of stimuli into modern functional devices without affecting the device performance, most probably due to the poor compatibility between stimuli, active materials and processing technologies. On-chip micro-supercapacitors (MSCs) are one kind of new-generation micro-sized power sources and have attracted considerable attention due to their small size, controllable patterning, in-plane feature and outstanding electrochemical performance. We will also demonstrate the fabrication of the stimulus-responsive and flexible MSC (SR-MSC) from our group.

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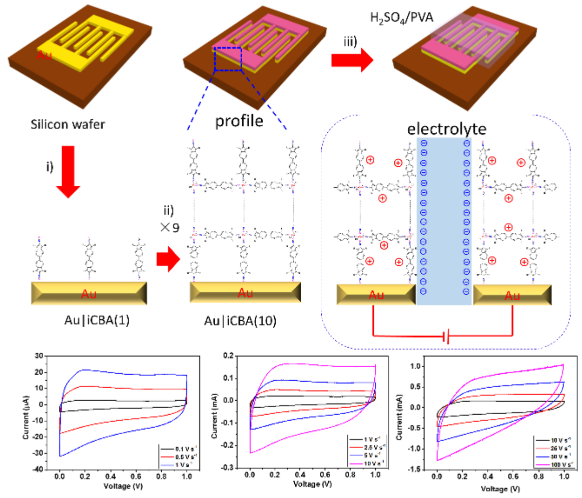

Figure 1. Coordination polymer framework based on-chip micro-supercapacitors with AC line-filtering performance.[1]

TNT2017 Orals – Seniors contributions

Challenges and Insights by Electrical Characterization of Large Area Graphene Layers

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Abstract

The current advances in the research and manufacturing of large area graphene layers are promising towards the introduction of this exciting material in display industry and other applications that benefit from excellent electrical and optical characteristics (cf. figure 1). New production technologies in the fabrication of flexible displays, touch screens or printed electronics apply graphene layers on non-metal substrates and bring new challenges to the required metrology. Traditional measurement concepts of layer thickness, sheet resistance and layer uniformity are difficult to apply to graphene production processes and are often harmful to the product layer. New non-contact sensor concepts are required to adapt to the challenges and even the foreseeable inline production of large area graphene. [1]

Dedicated non-contact measurement sensors are a pioneering method to leverage these issues in a large variety of applications, while significantly lowering the costs of development and process setup. Transferred and printed graphene layers can be characterized with high accuracy in a huge measurement range [2] using a very high resolution (cf. figure 2 and 3). Large area graphene mappings are applied for process optimization and for efficient quality control for transfer, doping, annealing and stacking processes. Examples of doped, defected and excellent Graphene are presented as quality images (cf. figure 4) and implications for manufacturers are explained [3] [4].

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Figures

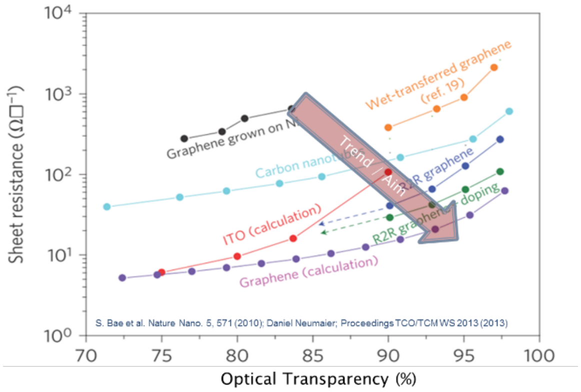

Figure 1. Achievable sheet resistance to optical transparency performance of Graphene and ITO

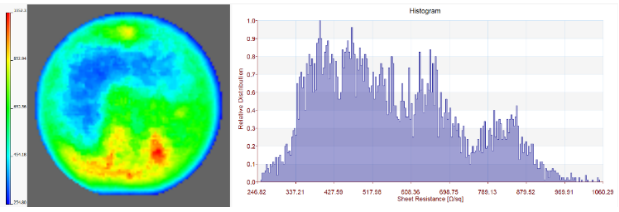

Figure 2. 4 inch Graphene showing handling defects

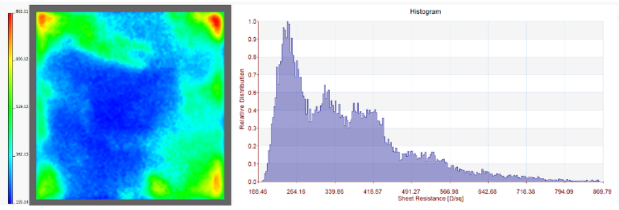

Figure 3. 6 x 6 inch Graphene transferred on PET with transfer defects

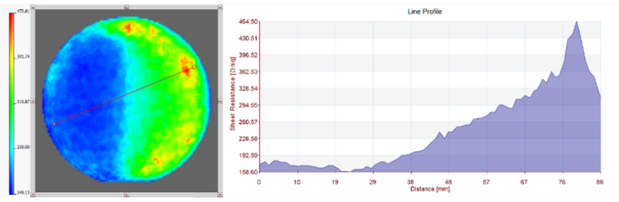

Figure 4. 4 inch Graphene with strong doping profile

First principle investigation on thermoelectric properties of transition metal dichalcogenides: Beyond rigid band model

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Two-dimensional direct band-gap transition-metal dichalcogenides (TMDC) with chemical composition MX_2 (M=Mo or W and X=S or Se) have led to a growing interest in the last decade. For instance, in the field of nanoelectronic, significant accomplishments have been done in the development of MoS_2 based transistors.

We have investigated the thermoelectric properties (electrical conductivity, Seebeck coefficient and power factor) of single layer TMDC on the basis of *ab initio* quantum transport using Landauer Büttiker formalism (see **Figure 1**). The often used rigid band model is compared to realistic doping, namely substitution and adsorption, it is found that several important physical insights governing the transport are missing in this approximation. The rigid band model appears to clearly overestimate the thermoelectic efficiency, hampering its relevance for thermoelectric studies. Substitution doping by chloride or phosphorus leads to poor power factor due to drastic changes of the pristine band structure. In contrast, adsorption doping by alkalies (Li, Na, K and Rb) favors larger power factor (see **Figure 2**).

Thanks to the landauer formalism, a realistic treatment of the disorder induced by the dopants is also investigated and reveals that Cl doping leads to very short localization length of 3.5 nm whilst K comes with micrometer length scale. The Anderson localization phenomenon in thermoeletric properties of single layer transition metal dichalcogenides definitely comes out as a main issue.

Figures

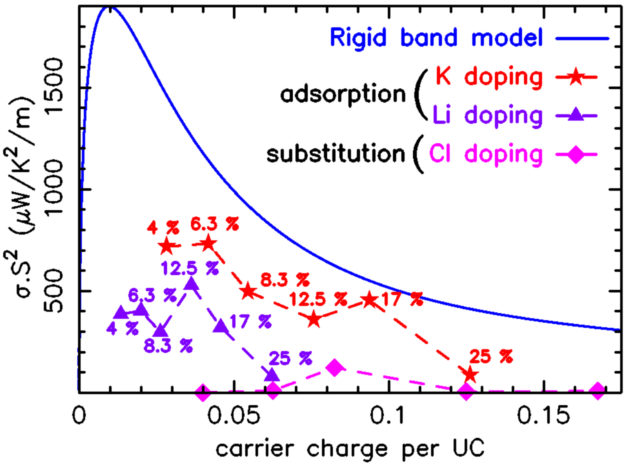

Figure 1. Schematic representation of the system within the Landauer formalism

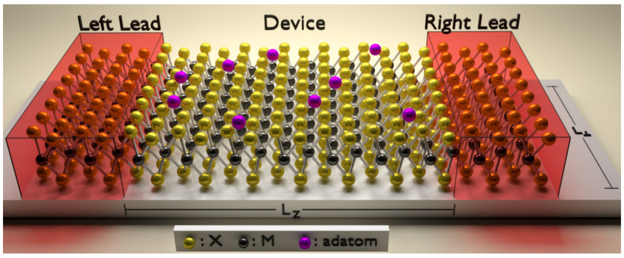

Figure 2. Power factor for MoS_2 with 3 different dopants: K, Li and Cl, as well as the rigid band calculation

Compact nanowire sensors probe emulsion droplets

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The fast evolution of high performance automated laboratory tests, point of care (POC) approaches for medical diagnostics [*1*], and smart routes towards new logic for chemical information processing [*2*] is to great extent driven by the smart combination of *microfluidics* and *nanotechnology*. In particular, droplet-based microfluidics (or digital microfluidics) - a versatile approach for operating a large amount of same size reactors in parallel is of particular interest, since it allows extremely parallelized and fine-tuned measurements, surpassing the precision of conventional assays. Although making an important contribution to classical detection and characterization laboratory assays, the application of droplet microfluidics in the spirit of miniature and light weight devices for *e.g.* POC applications remains a work in progress. The main impeding factor is related to the need for development and integration of novel *miniaturized optics-less* detection principle, outperforming the conventional approaches in terms of *e.g.* dynamic range or use of molecular labels.

Here we demonstrate a first combination of droplets microfluidics with the compact silicon nanowire field effect transistor in the microfluidic channel for ultrasensitive in-flow electrical detection of aqueous reactor-drops (Figure 1). Apart from detection events, we chemically probe the content of numerous (~104) independent reactors in a row, and resolve the pH values and ionic strength of the encapsulated solution, resulted in a change of a source-drain current through the nanowires. Optic-less and noninvasive measurements of these parameters in aqueous droplets can have a great impact on the area of biodetection and bioanalytics, where chemical processes performed in liquid environment are associated with the change of ionic composition or pH value in a medium. Finally, we demonstrate on a proof of concept level the GOx assay in droplets (enzymatic decomposition of glucose by glucose oxidase), measured simultaneously by SiNW FET sensor and integrated optical detector. Such realization of dual detection (SiNW sensor and optical luminescence) is demonstrated for the first time to the best of our knowledge [*3*].

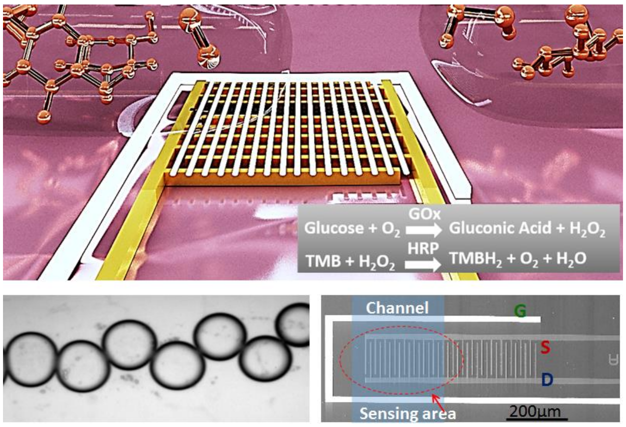

Figure 1: Conceptual description of the first combination of droplets microfluidics with the compact silicon nanowire field effect transistor in the microfluidic channel for ultrasensitive in-flow electrical detection of aqueous reactor-drops

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Intramolecular variation of spin-polarization within single molecule-surface hybrid

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Traditional single-molecule spintronics deals with magnetic molecules showing single-molecule magnet (SMM) properties adsorbed on non-magnetic surfaces [1,2]. Major challenges are (i) designing SMMs with sufficiently high blocking temperatures and (ii) controlling the molecular adsorption such that the molecules remain intact and maintain their key electronic and magnetic properties. In spite of extensive research, at present the achieved blocking temperatures do not exceed several tens of Kelvin.

We discuss an alternative approach based on aromatic molecules adsorbed on ferromagnetic surfaces. The chemisorption is governed by strong hybridization of molecular π-orbitals with *d*-orbitals of the substrate. The spin-split band structure of the latter leads to different hybridization for spin-up and spin-down states. This **spin-dependent hybridization** induces a spin-imbalanced density of states in the adsorbed molecule, which results in an induced moment for strong and spin-filter properties for weak coupling [3]. The hybridization also modifies the magnetic moment, exchange interaction, and anisotropy of the involved substrate atoms leading to magnetic hardening [4], *i.e.* these atoms and the molecule form a **hybrid molecular magnet** with enhanced coercivity and blocking temperature, *e.g.* above 240 K in Ref. 3.

Here, we study single triphenyl-triazine (TPT) molecules adsorbed on two layers of Fe on W(110) by **spin-polarized STM** (SP-STM) and density-functional theory (DFT) [5]. The adsorption of 3-fold symmetric TPT on the 2-fold symmetric substrate results in different bonding and hybridization conditions for the three phenyl groups in each TPT as directly evidenced by STM topography images. SP-STM data of single TPT adsorbed on different magnetic domains of the Fe/W(110) substrate reveal a hybridization-induced molecular spin polarization opposite to the surrounding Fe film, which varies on a nm-scale due to locally different binding conditions and hence confirms the concept of spin-polarized hybridization [6].

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Figure

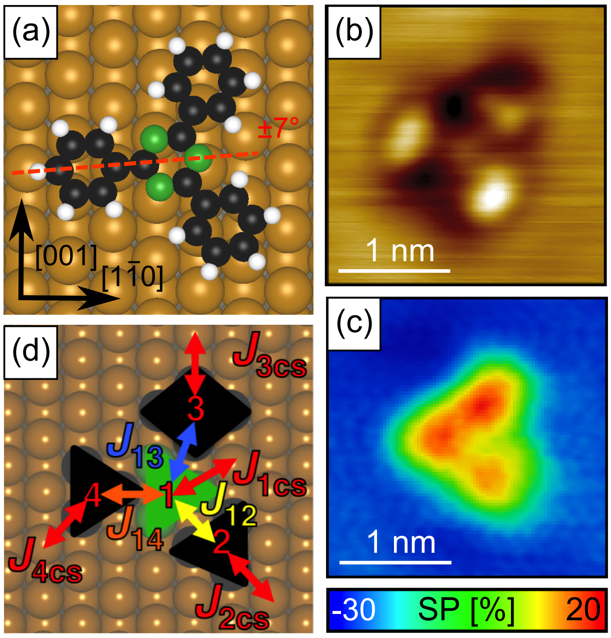

Figure 1. TPT molecule on two layers of Fe on W(110): (a) adsorption geometry, (b) STM topography, (c) spin polarization map, and (d) intramolecular magnetic subunits with their exchange couplings.

Rational Design of Graphene-Based Materials for Supercapacitors

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Energy storage systems such as electrical doublelayer capacitors (a.k.a. supercapacitors) are essential components of the renewable energy paradigm. Today, the widespread use of carbón materials as electrodes of supercapacitors is justified, for instance, by their remarkable electrical conductivity, chemical stability and wide range of operating temperatures. Still, current technology has not yet approached the maximum theoretical capacitance for pure carbon-based electrode materials (550 F/g) [1]. While recent literature has repeatedly investigated the use of chemically exfoliated graphene for supercapacitors [2,3], a systematic study on how different synthesis strategies affect the structure and chemistry of reduced graphene oxide (rGO) is missing. Likewise, steps such as the drying methodology have been mostly overlooked.

In this presentation, I will describe our strategy to rationally approach the synthesis of rGO materials [4,5] and how this enabled considerable improvements in electrochemical capacitance. We observed that, besides a judicious selection of the graphite's oxidation–reduction route, it is critical to control the final drying step. Through it, one can significantly increase the specific surface area of the rGO powder and preserve its porous network (Fig. 1), thereby maximizing the supercapacitance performance. In these circumstances, while previous studies on hydrothermally reduced GO invariably reported low surface area (<100 m^2/g) and capacitance (<300 F/g) (cf. for instance ref. [3]), we achieved unprecedented values of 364 m^2/g and 441 F/g, respectively. [6]

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Figures

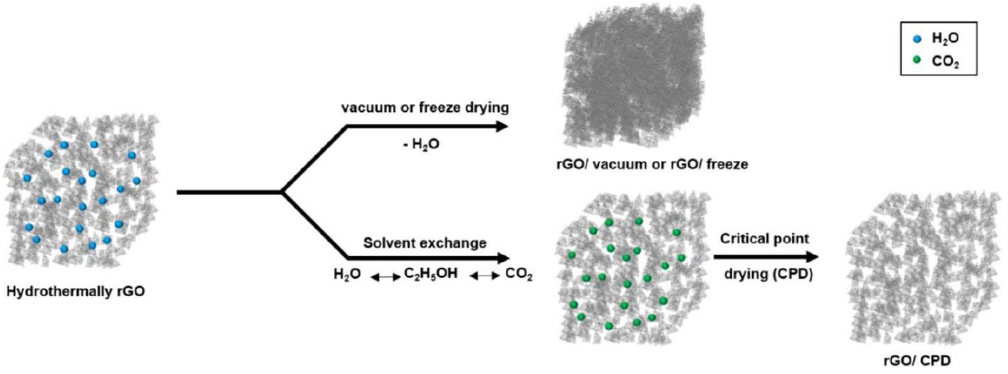

Figure 1. Schematics of the various drying processes that were investigated.

Novel Drug-Templated Mesoporous Silica Nanocontainers and Protocells Based Thereon

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Mesoporous silica nanoparticles (MSNs) are of significant interest as nanocontainers for different substances, primarily – for drugs [1]. Conventional route to use of such nanocontainers includes several stages: 1) sol-gel synthesis of MSNs using the micelles of "*inert*" surfactant as a template, 2) template removal, 3) modification of inner and/or outer surface of the MSNs (this allows one to control the sorption/desorption kinetics of a drug), 4) drug loading. This route results in low drug uptake and burst release that are insufficient for the most applications.

We propose a new approach that overcomes these drawbacks. This approach is based on the use of micelles (or vesicles) of the *targeted substance itself* (instead of *inert* surfactant ones) as templates at MSNs synthesis. As a result, it becomes possible to combine the stages of silica nanocontainers synthesis and their loading with the targeted substance.

The prospects and benefits of such route are exemplified by the encapsulation of various bactericidal drugs (including cleavable ones) and an antitumoral agent. It is shown that the synthesized nanocontainers are characterized by an extremely high capacity with respect to templating functional compound (about 1 g and over per 1 g of SiO_2) and are also pH-sensitive.

The effects of the template nature and conditions of the sol-gel process on the porous structure of silica vehicles are studied and discussed.

The kinetics of the template molecules' release from the silica nanocontainers is studied and some features of this process are analyzed.

We also discuss the possibility of such particles use as a basis to creation of protocells – fundamentally new means of drug delivery.

This work was financially supported by RFBR (Project no. 16-03-00118).

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Interfacial Synthesis of 2D Polymers and 2D Supramolecular Polymers

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At present, one of the key challenges faced by the scientific community is to go beyond graphene. The two-dimensional polymers and two-dimensional supramolecular polymers (2DPs and 2DSPs: laterally infinite, one atom- or monomer-unit thin, free-standing, covalent and noncovalent networks with long-range order along two orthogonal directions, respectively) have recently emerged as a new class of 2D materials and exhibit intriguing physical and chemical properties. Here, we present the bottom-up synthesis of 2DPs and 2DSPs towards large-area, free-standing feature, high crystallinity, tunable pore structures, and controllable thickness (from single-layer to multilayers) by reliable interfacial synthesis strategies (such as air/water (Figure 1), liquid/liquid interfaces) and chemistry methodologies involving of host-guest interaction, metal-dithiolene/-diimino coordination reactions, and imine/imide dynamic covalent reactions.[1-6] Notably, proof-of-concept applications of such 2DPs and 2DSPs suggest they are promising materials in energy storage and conversion, sensing, catalysis and membrane, and are expected to pay the way for the development of new generation of organic electronics.

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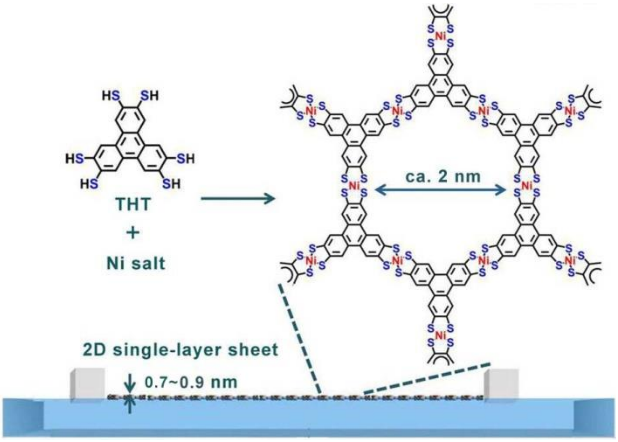

Figure 1. Schematic illustration of bottom-up synthesis of graphene-like 2DSP at air/water interface.

Towards prediction of *in vivo* behavior of nanoparticles: A quartz crystal microbalance platform for characterization of nanoparticle - cell interactions in a complex biological milieu.

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When nanoparticles (NPs) enter a biological milieu, they come into contact with a huge variety of biomolecules including proteins. These proteins immediately coat the NP surface and form a protein corona. As a consequence, the original “synthetic identity” of the NPs is covered by the corona and a distinct “biological identity” is acquired. This new corona identity governs how the NPs are “seen” and subsequently interact with cells and other bio entities. Yet, it is not clear how the physical and chemical properties of NPs affect the composition and structure of the protein corona and, in turn, cellular interactions. Improved understanding of the interaction mechanisms and the response of living systems to NPs can accelerate the implementation of nanotechnologies in medicine. We have developed a label free dynamic flow QCM-based platform and methodology for characterization of the bio-nanointerface. This enables identification of key molecular details for NP interactions with cells. A “library” of core and functionalised nanoparticles has been employed to understand the link between NPs physicochemical properties (size, shape, surface chemistry and functionalisation) and the functional protein epitopes of the corona that generate the biological recognition on the surface of the particles. The platform allows studies of the effect of surface modifications of NPs on the interactions with cells grown on QCM sensor surfaces. The results highlight fundamental relationships between NP design, the protein corona, and cellular interactions and demonstrate the potential of the platform to predict NP-cell interactions within a biological system.

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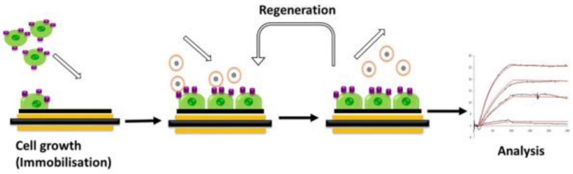

Figure 1. Experimental set-up

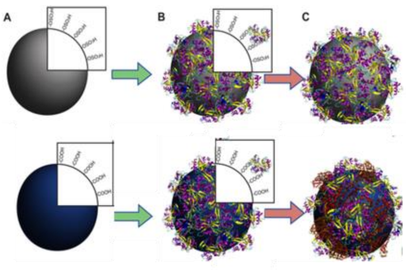

Figure 2. PS NPs modified with sulphonated groups (upper) and carboxylic groups (down) coated with transferrin by physical adsorption

Magnetron Sputtered WS2 Thin Films

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The Unique optical and electrical properties of 2D materials permit many important device applications. One of the most well-known 2D material, graphene attracts attention for semiconductor device applications due to its strong interaction with photons in a broad wavelength range and its high carrier mobility [1-3]. However, field effect transistors produced from graphene cannot be effectively switched off and have low on/off switch ratios due to lack of bandgap [4]. This brings up the importance of other 2D materials at least for the transistors applications. These 2D semiconductors are Transition Metal Dicalcogenides (TMDCs) given by the MX2, M;transition metal (Mo, W, i.e) and X; chalcogenide (S, Se, i.e) [4]. Best known 2D semiconductors materials are MoS2, WS2, MoSe2, WSe2. These materials show very important properties such as indirect-to-direct band-gap transition from monolayer to bulk regime, coupled spin and valley physics, and band structure tunability with strain. Furthermore, the combination of WS2 thin layers with other 2D materials has given rise to a large category of 2D hetero-structures. Changing its properties mainly from a single layer to thick layers makes these materials very suitable for in-situ structural analysis.

Thin films of WS2 were grown by radio frequency magnetron sputtering (RFMS) down to a few layer to 700 nm on different type of substrates in different growth conditions. Effects of growth conditions, such as RF power, temperature of the substrate, thickness, different type of substrates, on the grown thin films were investigated by X-ray diffraction (XRD), X-ray Photoelectron Spectroscopy (XPS), Raman Spectroscopy (RS), Atomic Force Microscopy (AFM), Photoluminescence (PL), and optical absorption measurements. XRD studies showed that growth conditions have huge impact on the material's crystal quality. Peak belong to (002) plane appeared commonly grown at higher RF powers and thicker samples. In addition to the observation of the (002) plane, (10l) and (11l) (l=0,1,2,3) peaks was observed in all of the thin films. Raman scattering measurements showed signal coming from two modes, namely 352 cm-1 and 418 cm-1 corresponding to E2g1 and A1g modes from in plane and out-of plane vibrations, respectively. Binding energy depth profile for W4f7/2 and W4f5/2 is represented for the thin films grown at different condition which showed two satellite peaks settled at 31.5eV and 33.8eV. Deconvolution of the spectrum is to a doublet consisting of S 2p3/2 and S 2p1/2 peaks centered at binding energy values of 161.88eV and 163.18eV. Optical absorption of the films give rise to a 1.2 eV bandgap energy while it is changing when the thickness decreases

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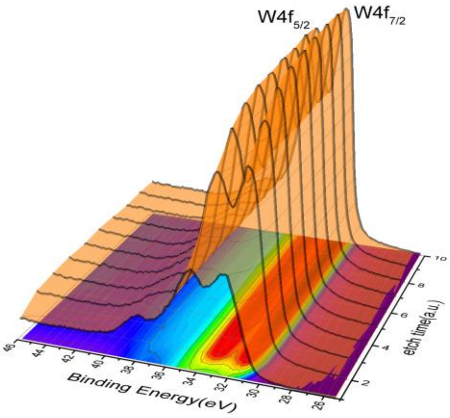

Figure 1. XPS depth profile of the W4f

A Targeted Functional Design for Highly Efficient and Stable Cathodes for Rechargeable Li-Ion Batteries

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Despite the great success of the Li-ion batteries (LIBs) up to now, higher demand has been raised with the emergence of the new generation electrics, such as portable devices and electrical vehicles.[1] Even with the improvement on anodes, the cathodes with high capacity and long-lasting remains a challenge. A new 3D $NiCo_2O_4@V_2O_5$ sandwich arrays (SAs) on Carbon cloth as cathodes in LIBs is reported in this work.[2] The nano-designed materials realized the theoretical specific capacity of V_2O_5 with high power rate, ~ 292.0 mAh g^{-1} at the current density of 0.1 C, based on the total mass of the framework and amount of active materials. The electrodes achieved superb cycling stability, 0.0126% capacity decrease per cycle within 500 cycles at the high current density of 10 C, among the most stable cathodes for LIBs ever reported. From both in-situ TEM and quantum level calculations, the 3D $NiCo_2O_4$ nanosheets frameworks provided high electron conductivity and the skeleton of the robust SAs without participate the lithiation/delithiation; the thickness of the layered V_2O_5 plays a key role for Li diffusivity and the capacity contribution of electrodes. The structures herein point to new design concepts for high-performance nanoarchitectures for LIB cathodes.

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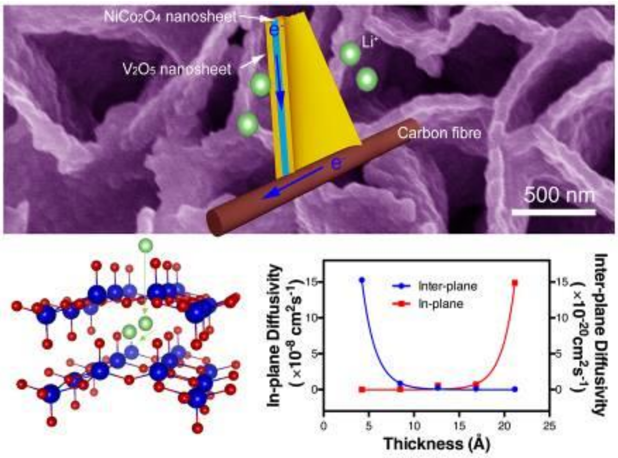

Figure 1. Nano-architectured cathodes materials for lithium ion batteries are introduced. The high capacity and stable characteristic routed from the bi-pathway design of electron conduction (the core material) and lithiation/delithiation reaction (the shell material). Further optimized thickness of the shell to balance the capacity and Li diffusivity efficiency was studied from both experimental and theoretical approaches.

Ebola biosensing with a gate controlled memristor mode

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Nanowire-based field-effect transistors (FETs) are currently attracting a strong attention due to their potential to deliver promising miniaturized diagnostic tools with a high and label-free sensitivity [1,2]. Recently, the use of their memristor property was demonstrated as biosensing principle, showing that the binding of charged biomolecules bring a violation of its zero-crossing signature by opening a voltage gap V_{GAP} in the current minima when the source-to-drain voltage V_{SD} was swept [3]. The demonstration was done in dry conditions to get rid of the screening effect caused by the excess of nonspecific ions.

In this work, we demonstrate the biosensing in the memristor mode directly in a liquid environment using a FET based on a pattern of honeycomb shaped silicon nanowires (Figure 1a). We engineer the gap opening process by applying a gate voltage V_G through the reference electrode that mimics the presence of surrounding charged species of the desired sign (Figure 1b). An initially opened gap V_{GAP} allows to detect the biomolecules carrying arbitrary, positive or negative charge that results in either further increasing or closing the V_{GAP}, respectively. The VP40 matrix protein from Ebola virus is detected in a miniaturized electronic nanobiosensor for the first time, in femtomolar levels, by analyzing the needed V_G to maintain a constant value of V_{GAP}=1.5V (Figure 1c). We finally compare the same device performance in terms of its detection range and sensitivity to the results obtained in the already known field-effect transistor (FET) mode (Figure 1d), showing that the memristor mode is sensitive at the same concentration levels as the FETs.

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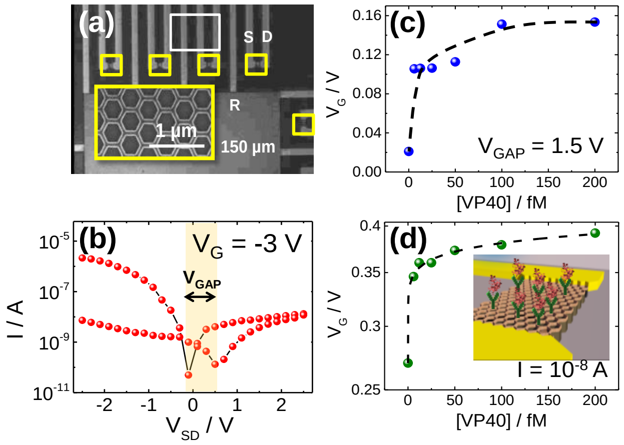

Figure 1. (a) Nanosensor where S=source, D=drain, and R=reference denote the electrodes. The inset shows silicon nanowires located at yellow areas. (b) A V_{GAP} opening (orange area) appears by applying a negative V_G. (c) The biosensing in the memristor mode. At increasing protein concentrations, V_G needs to be increased in order to maintain a constant V_{GAP}=1.5V. (d) The biosensing in the FET mode. The inset depicts the device modified with antibodies that catch the target protein.

Photosynthesis; Miracle of Organic Life and its Technologies

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Photochemical reaction carbon dioxide, nitrogen and water in at our atmosphere, production of amino acids, following protein molecular structures, finally creation of micro-living species, and the birth of plants, animals! These microscopic molecular structures (*in rivers, lakes, seas*) had given birth to moss on land, further all sorts of plants, animals and human beings, that is called as the Miracle of Universe

$$6n\,CO_2 + 6n\,H_2O \xrightarrow{hv} (C_6H_{12}O_6)_n + O_2 + \text{ısı}\,(\Delta E)$$

Consumption of fosile fuels over millenia, now had given birth to atmospheric enhancement of heat, variation of seasons and exhaustion of limited energy sources. As a result, conversion of solar energy into electricity is now a most attractive technology. As known, miracle of photosynthesis, provides the energy needs of all living species on our Earth.[1,2]

On the other hand, in last quarter of century, Organic Photo-Electronic Technolojigies of OLED, OFET, OPV, entered rapidly to our daily life.[3-5] A distinct example is OLED-Organic LED lamps. Mobile phones, Lap-Top Computers, colored TVs e.t.c. were based on OLED technology[6]. Of course, these developments on Organic Technologies, are steps to adaption of human kind into nature, leaving the emoployment of steel, iron and birghtons our future centuries.[1] The OLEDs and fllowing the OPV-Organic Photo Voltaics and OFET-Organic Field Effect Transistors, entrering into all of our elektronic systems, capable us compatability of our technological systems-tools into nature, and our Earth will not be threatend by poisonous waste problems, our running waters will be drinkable-washable.

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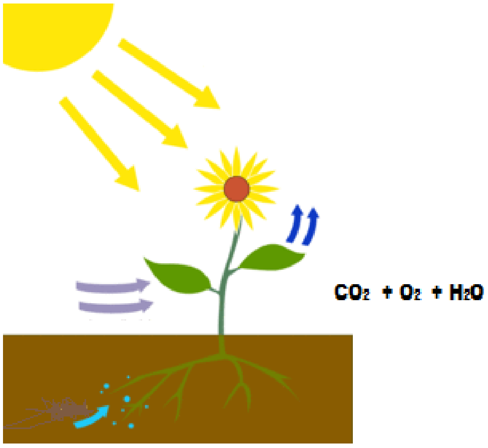

Figure 1. Photosynthesis.

Bifunctional Porous Nanomaterials for Cell-Biomaterial Interaction Studies

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Multifunctional porous nano(micro)meter-scaled materials (NMs) that combine several specific properties (e.g., magnetic, optical, bioactive) have found many applications in biomedical fields such as drug delivery, diagnostic, magnetic resonance imaging, bioseparation etc. The assemblies of such functional NMs on substrate surfaces (arrays of NMs) or in hydrogel networks [nanocomposite (NC) hydrogels of NMs] have been used especially as 2D and 3D biomaterial surfaces to mimic extracellular matrix (ECM) and to study cell-material interactions.[1]

In this context, we use porous NMs, for the preparation of (gradient) 2D and 3D biomaterials to study cell-material interactions and for controlled drug delivery applications (Figure. 1). We describe the external and internal surface functionalization of NMs with (chiral) bioactive molecules and fluorescence dye molecules, respectively,[2] preparation of their arrays[3] and NC hydrogels[4] for controlled cell adhesion and migration, cellular patterning, and chirality-dependent cell enrichment and cell-cell separation.[3-7] Our results demonstrate that different types of cells have different adhesion and proliferation behaviors on the arrays of bifunctional NMs with respect not only to the type of the used bioactive molecules,[2,4,6] but also to the enantiomers of bioactive molecules showing the stereoselective interactions between cell-biomaterial surfaces.[3,7] Additionally, we use functional NMs as nanocontainers to deliver model drug molecules to cells as a proof of principle for controlled drug delivery.[4,7,8]

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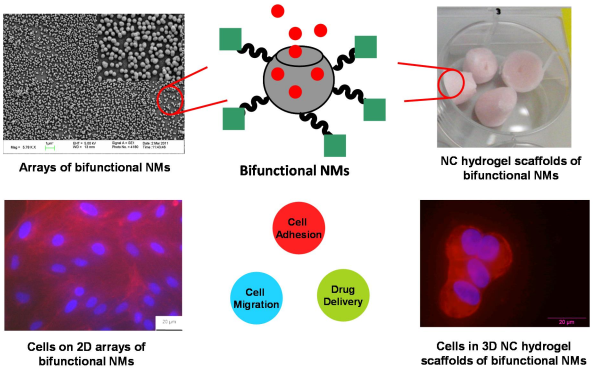

Figure 1. Arrays and NC hydrogels of bifunctional NMs for cell-biomaterial interactions.

Nitrogen and Sulfur Co-doped Holey Graphene Aerogel For High-performance Compression-Tolerant All Solid-State Supercapacitors

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Deformation-tolerant power-source devices are crucial for designing high-tech elastic electronics owing to their elasticity of integration into preferred levels of eccentric forms while maintaining the performance and reliability.[1] Among various power-source devices, compression-tolerant all solid-state supercapacitors (ASSCs) could be a strong candidate for next-generation elastic electronics.[2] However, the use of non-conductive compressible substrate and pseudocapacitor agents as additives could inhibit the compressibility as well as the performance of the devices. Therefore, proper selection of porous foam-like electrodes with remarkable compressibility, sustainable conductivities and electrochemical performances under verying compressions are the critical prerequisites to develop high-performance compressible ASSCs. Here, we introduce a facile technique without using any additives for fabricating highly compressible, electrically conductive, nitrogen and sulfur co-doped holey graphene aerogels (NS-HGA) as an efficient electrode for high-performance compressible ASSCs. Such covalently interconnected holey framework with heteroatom co-doping greatly increases repeatable elasticity and excellent structural robustness, high electrolyte ion storage ability, unimpeded ion channels to offer excellent conductivity (21.66 S m^{-1}) and significantly high volumetric capacitance (203 mFcm^{-3}) in ASSCs with good rate capability and almost unaltered capacitance at 50% compression with good durability for 200 cycles. The current unique methodology to develop heteroatom co-doped holey graphene aerogel for designing high-performance compressible ASSCs will pave a new approach in the modern era of elastic electronics.

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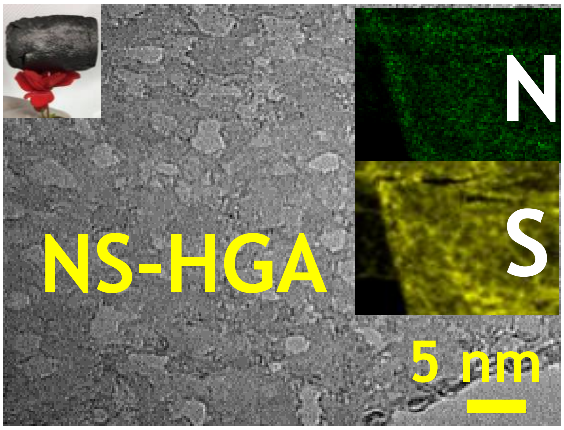

Figure 1. HRTEM and STEM images of N and S co-doped ultra-light graphene aerogel

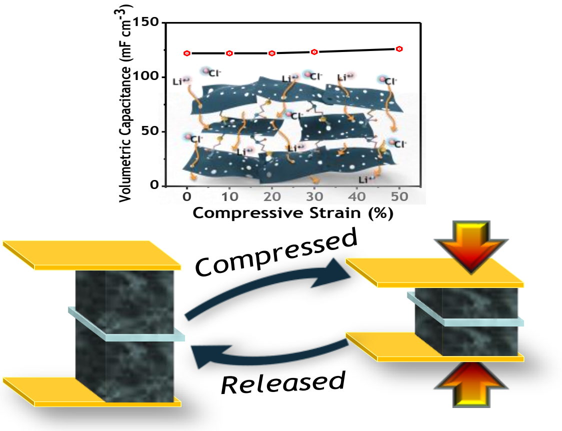

Figure 2. Compression-tolerant all-solid-state supercapacitors

One-atom-thick 2D material based on CuO. Experimental observations and theoretical study

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2D materials have attracted lots of attention since discovery of graphene which was found to exfoliate easily from bulk graphite. Increasing of such interest has recently triggered for the study of two-dimensional materials with nonlayered bulk like boron, zinc oxide, sodium chloride or iron. Among all these materials the latter one attracts special attention because the formation of two-dimension layered metal is unexpected and controversial due to the indirect nature of metallic bonds.

In this work we present the observation of novel two-dimensional one atom thick layer based on copper oxide studied by both experimental and theoretical methods.

Using *in situ* STEM it was observed special crystal lattice of 2D CuO on graphene which structure is principally different from the former reports. Structural parameters and chemical compounds of 2D cluster were determined.

Using DFT the stability and properties of observed CuO nanoclusters was studied. It was defined a critical role of the oxygen impurity atoms in the formation of stable 2D CuO cluster with unexpected orthogonal crystal lattice. Mechanical, electronic and magnetic properties were studied as well.

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Figures

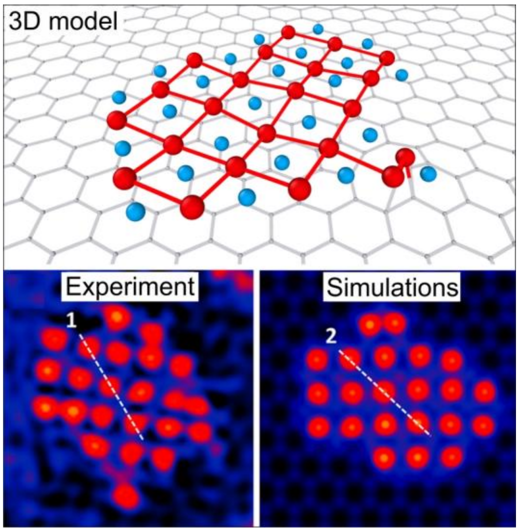

Figure 1. Atomic model of observed CuO cluster (top panel); STEM image in comparison with simulated STEM image of the sample (bottom panel)

Ordered Non-Covalent Functionalization of Graphene by Controlled Formation of 2D Supramolecular Self-Assemblies at the Graphene Surface Forming Hybrid vdW Heterostructures

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The rise of graphene and related 2D materials makes possible the formation of heterostructures held together by weak interplanar van der Waals (vdW) interactions.[1,2] Periodic potentials naturally occur at the interface, which can significantly change the electronic structure of the individual materials within the stack, thus offering the possibility to build up novel structures with unique properties. Unfortunately, it is quite hard to precisely control the periodic potential in these structures since they are essentially determined by the lattice mismatch between the different materials.[3,4] Also, the fabrication of such inorganic vdW heterostructures is quite demanding in terms of technical efforts and costs. In this context, combining different molecular functionalities in a same graphene heterostructure is highly attractive for several reasons. First, graphene can be doped with a variety of molecules, which can act as nanoscopic potentials and locally modify graphene electronic structure.[5,6] Secondly, crystalline structures with 2D architecture can be formed with a collection of molecules capable of physisorbing on graphene and other 2D materials.[7,8] In this regard, self-assembly of linear alkyl chains is particularly interesting. As a matter of fact, it is now well established that long alkane chains, and related functionalized molecules physisorb on graphite surface, generating highly ordered 2D patterns.[8,9] Besides, periodic modulation with different geometries are predicted to affect the electronic band structure of graphene in very different ways. Namely, an anisotropic propagation of the charge carriers is predicted for graphene sheet in which a 1D potential is applied.[10]

Here, we explore the 1D modulation of graphene properties that is programmed with atomic precision via the exploitation of self-assembled monolayers driven by linear alkyl chains, generating well-organized supramolecular architectures at the graphene surface.[11]

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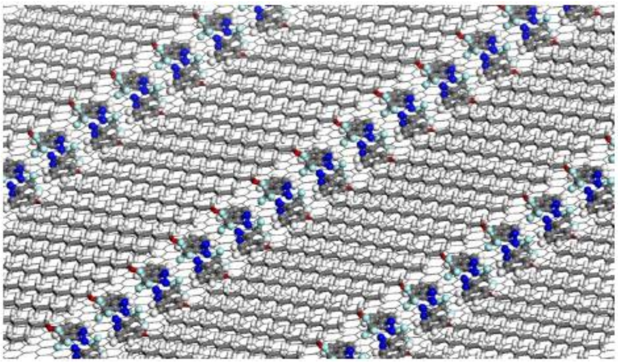

Figure 1. Self-assembled monolayer physisorbed at the graphene surface. The molecules are made of a long alkyl chain, which drives the self-assembly at the graphene surface, forming highly ordered supramolecular structure.

Ultrasmall nanoparticles for bioapplications: potential in droplets based microfluidics

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Recently, ultrasmall nanomaterials (sub-10 nm size) have started to attract increasing attention due to their properties and their potential for medicinal applications [1]. In this direction, ultrasmall silicon nanoparticles (Si NPs) and carbon dots (CQDs) are gaining in importance, especially in the imaging and therapy [3, 4] of e.g. cancer cells. Both types of particles display photoluminescence, high resistance against photo-bleaching, chemical stability after functionalization and biocompatibility. The possibility to modify their surface in a covalent way, render them an advantageous platform to anchor targeting therapeutic drugs and/or labels (red-emitting dyes for optical imaging, bifunctional chelator agents for e.g. radiometals enabling SPECT or PET).

The interactions of this kind of NPs with cells using novel *in vitro* techniques, such as droplets based microfluidics/millifluidics, offer new perspectives. Indeed, due to the automated continuous monitoring of the fluorescence signal [5], cells can be studied for long times and in a controlled way. This would help to implement the state-of-the-art of cells/nanoparticles interactions by creating a more realistic representation of *in vivo* conditions in 3D isolated environments, such as droplets, with the opportunity to perform many simultaneous experiments and the chance to reduce the number of *in vivo* experiments.

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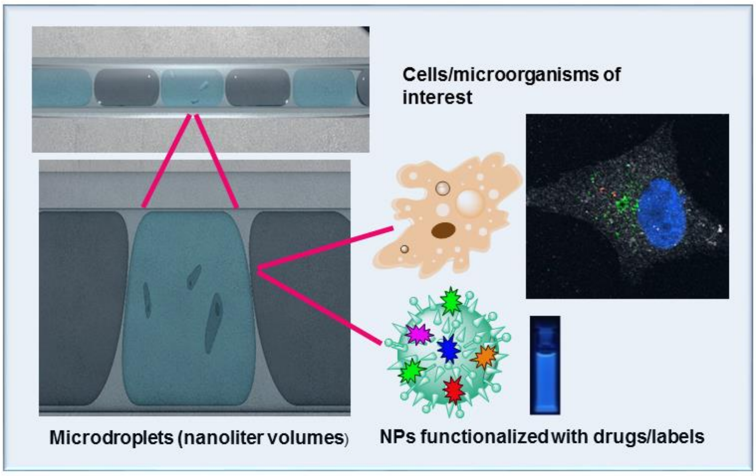

Figure 1. Cells/microorganisms and properly functionalized NPs inmicrodroplets (nanoliter volumes).

Monolithic Cobalt Phosphide Nanowire Electrodes for Efficient and Durable Water Splitting

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Abstract

Hydrogen (H_2) is a promising energy carrier and has many advantages over hydrocarbons for use as a fuel for both stationary power and transportation. Water electrolysis has been proposed to be the cleanest way to produce H_2, because unlike steam reforming of hydrocarbons this process doesn't emit any pollutants and water is an inexpensive renewable resource. More importantly, H_2 produced from water electrolysis has high purity and is free of carbon monoxide, and therefore can be directly used to feed fuel cells without a risk of poisoning the anode catalysts.

Water electrolysis usually cannot be efficiently accomplished without a catalyst. Recently, metal phosphides have emerged as a new class of electrocatalysts that can promote both the H_2 evolution reaction (HER) and oxygen (O_2) evolution reaction (OER) [1-3]. In this presentation, a monolithic cobalt phosphide (Co-P) nanowire electrode will be presented, which were prepared by a simple one-step vapor-solid reaction method [4]. The obtained Co-P nanowire electrodes exhibits excellent electrocatalytic performance for both HER and OER as well as overall water splitting. Significantly, the electrode can sustain upon long-term water electrolysis for up to 1000 h without degradation, showing extraordinary operational stability.

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Figures

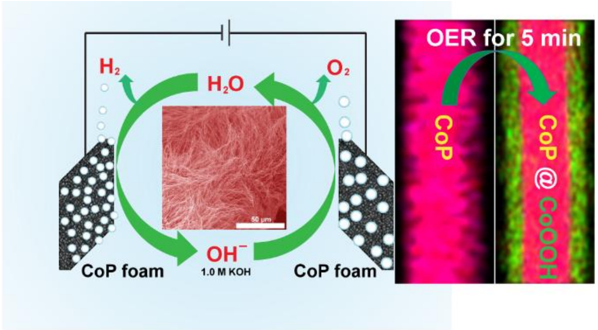

Figure 1. (left) A scheme showing overall water splitting using two symmetrical monolithic Co-P nanowire electrodes as anode and cathode. (right) STEM elemental maps of a single Co-P nanowires showing the conversion of phosphide to oxyhydroxide upon the OER.

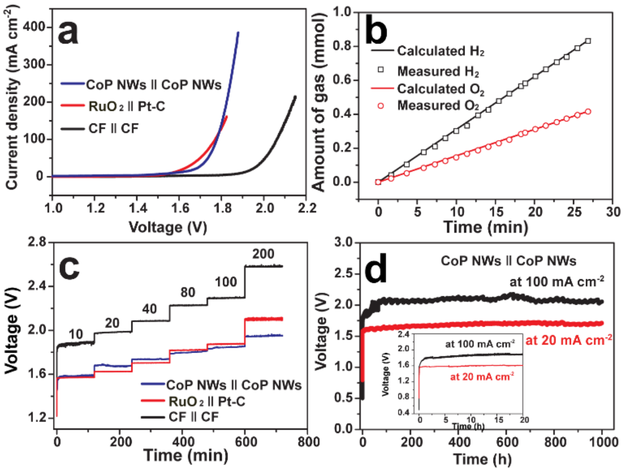

Figure 2. Overall water splitting performance of the two-electrode Co-P NW electrolyzers.

Using single nanoparticle tracking to simultaneously characterize nanoparticle size distribution and nanoparticle-surface interactions

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Measuring and understanding the interactions between nanoparticles (NPs) and cell surfaces, are of paramount interest for the developing specific targeting drug delivery complexes based on NPs. Experimentally, the direct measurement of the forces between nanoparticles (NPs) and surfaces by traditional methods (e.g. AFM) in realistic exposure conditions is challenging due to that these interaction occur in complex environments (usually under fluid flow conditions, at high salt concentrations, at room temperature, etc). As an alternative, in this work we present a novel technique to characterize NP-surface interaction in a microfluidic chamber. The proposed method is based on generating an optical potential to trap NPs close to a surface. A schematic representation of the experimental setup is shown in Fig. 1a. The main element of the device is a waveguide (WG) that transports light from a laser source through the experimental chamber. The propagated light generates an exponentially decaying field that extends above the waveguide. The NP will then go under Brownian motion and will scatter light. The closer to the WG the more light it will scatter (as the light intensity decays from the WG to the medium) and this effect is used to measure the fluctuations around the minimum of the potential well (Fig. 1c). Using a video camera, the position of the NP is recorded and a the full 3D trajectory is reconstructed as shown in Fig. 1b. Here we outline a further application of this technique to measure the size of single particles and based on these measurement build the distribution of a sample. We demonstrate its efficacy by comparing the size distribution obtained to established instruments, such as dynamic light scattering and differential centrifugal sedimentation. Our results were in good agreement to those observed with all other instruments. Furthermore, we demonstrate that the methodology developed in this work can be used to study complex particle mixtures and the surface alteration of materials. For all cases studied, we were able to obtain both the size and the interaction potential of the particles with a surface in a single measurement [1]. We also use the same methodology to study the effect of a coating layer on the diffusion silica NPs close to a surface [2].

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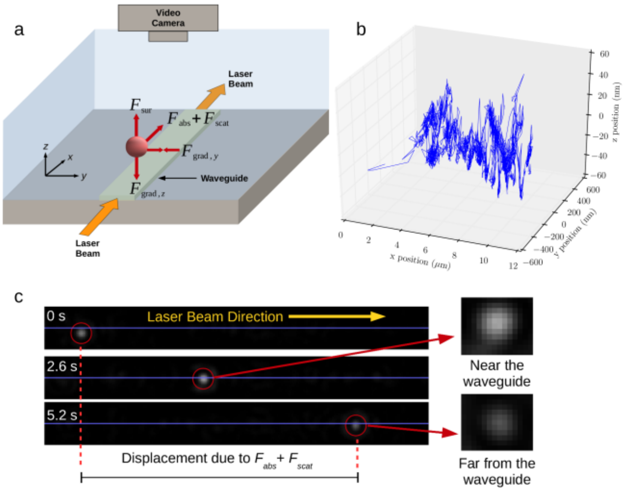

Figure 1. (a) Schematic representation of the experimental setup. (b) Full 3D trajectory of one NP. (c) Images of a NP traveling over the WG at different times. Due the exponential decay of the evanescent field, NPs closer to the surface scatter more light and are detected brighter. The direction of the light in the WG is from left to right and so is the movement of the NP.

From carbon shells to multipods - The role of nickel particle shape and size

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Abstract

The process of producing structured carbon nanofibers (CNFs) by decomposition of various hydrocarbons has attracted the attention of many researchers because of the unique properties of these carbon materials. The recent interest in CNFs and their potential applications emerges from their relationship to carbons with graphite like layers such as fullerenes and carbon nanotubes (CNTs), with particular focus on their synthesis[1,2]. However, control over the size and morphology of these materials still remains a challenge. It has been suggested that catalyst morphology plays an important role in controlling CNFs growth and its shape. Therefore one of the challenges is to produce catalyst particles that would yield the desired CNFs morphology. This study investigates the approach for controlling the size of CNFs by synthesizing metallic nickel nanoparticles (NPs) of particular morphology using microemulsion technique.

Trichloroethylene, acetylene and their mixtures were used as a carbon source to make CNFs over Ni nanoparticle catalysts in a chemical vapor deposition (CVD)[3] process in the temperature range 350-700 ^{0}C. TEM analysis of the Ni particles revealed that the Ni underwent a morphological change with increase time. Further, the shape of the carbon materials produced from the Ni catalyst was affected by temperature. The carbon shapes changed from carbon shells to bimodal, to tripod-like structures and eventually multipod-like structures with increase in temperature (350-700 ^{0}C). TEM image of a multipod-like structure is shown in Fig. 1. Irregular shaped materials were observed at temperatures greater than 500 ^{0}C. It was also found that when acetylene or an acetylene/trichloroethylene mixture was used at 450 ^{0}C, helical and linear fibers were produced. It was also demonstrated that H_2 had a dramatic influence on the morphology of CNFs. The results show that the catalyst morphology can be modified by the selective use of the carbon source to generate a wide range of carbon shapes.

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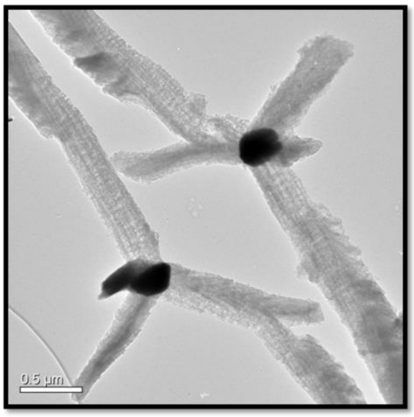

Figure 1. TEM image of multipod CNFs synthesised at 500 ^{0}C.

Electrical Conductivity and micro-Raman Sectroscopy of Graphene Layer Deposited on SiO_2 Dielectric and Subjected to Electron Beam Irradiation

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Modifying the properties of the carbon structures by radiation treatments attracts scientific interest as a promising method for the electronic properties tuning of the further nanoelectronic devices. This paper dedicated to the research of the electronic properties of the single layer graphene (SLG) subjected to the medium-energy electron-beam irradiation (EBI).

The SLG films had been grown by the CVD on Cu foil and transferred to the SiO_2(300 nm)/p-Si substrate. The Ni contacts (transfer length measurement set) were deposited on the SLG by the DC magnetron sputtering. The SLG region between Ni contacts was subjected by electron beam with energy of 20 keV with 1 A/cm^2 current density focused on an area of 2.5x 10^{-7} cm^2. Irradiation doses were in range from 1x10^3 – 7x10^3 μC/cm^2.

The micro-Raman spectra of initial graphene film measured between of the metal contacts showed prominent characteristic graphene peaks at 1580 cm^{-1} (G) and 2730 cm^{-1} (2D) along with a minor D peak at 1370 cm^{-1}. The peak intensity ratio (I_{2D}/I_G), which is 2.37 (average along of the film) with standard deviation of 0.68, is clearly indicating that the graphene has a monolayer thickness. Ratio of intensities of the D and G peaks indicates the quality of the material and for initial SLG film is 0.26 with standard deviation about 0.06. That is evidence of different defectiveness along of the film. Kelvin probe force microscopy (KPFM) technique [1] demonstrates heterogeneity of the film, which has a "grainy" structure with grain dimensions that approximately are 5-6 μm.

Frequency depended conductance measurements had been performed. The complete film conductivity σ could be represented as $\sigma = \sigma_{DC}+\sigma_{AC}(\omega)$, where σ_{DC} - is constant field contribution, $\sigma_{AC}(\omega) = A\omega^s$ - AC field contribution, that corresponds to Eliot model of hopping conduction [2]. The low-frequency (1-10 kHz) conductance σ_{DC} of the sample has decreased with irradiation dose up to 3 times. Carriers transport in AC field is limited by potential barriers (grain's boundaries) and intrinsic defects of the film (vacancies, dislocations). However, experimentally obtained values of power low ("s") are considerably higher then 1 for samples subjected to low-dose EBI, and at doses about 7x10^3 μC/cm^2 it decreses up to 0.26, that demands additional theoretical consideration.

The G line position of Raman spectra undergoes a blue shift , and full width at half maximum (FWHM) of the G line demonstrates narrowing with increasing dose up to 2x10^3 μC/cm^2, that can be associated with doping of the graphene layer [3]. A red shift of 2D line position with increase of irradiation dose attests electron doping of the graphene layer [3] that corresponds to positive charge generation in SiO_2 dielectric layer during electron beam irradiation. Additionally increase standard deviation for G line position along graphene channel with dose increase was observed that can be an indication on increase of doping fluctuation in graphene and can result in an increase of a carrier scattering in the graphene channel and reduction of graphene carrier charge mobility.

Thus, strong decrease of a conductivity of the CVD graphene layer on SiO_2 thin film at low-dose EBI probably associated with increase of a potential fluctuation in the SiO_2 layer and strong fluctuation of a charge concentration in the graphene layer.

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Design of artificial organelles by combining proteins with synthetic nanocompartments

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New concepts that combine multifunctional compounds with stable, safe carriers or membranes are on focus in a variety of domains, such as medicine, catalysis, environmental science, and technology. Suitable amphiphilic block copolymers are ideal candidates for applications because they can self-assemble into supramolecular assemblies, such as compartments, or planar membranes with a superior stability, and robustness compared to the lipid based membranes.[1] By combining these polymeric membranes with suitable biological entities, e.g., by incorporating integral membrane proteins or by enzyme encapsulation in polymer compartments it is possible to provide well-defined functions, such as molecular recognition, cooperation, and catalytic activity.[1]

Here, we present distinct spaces for desired reactions at the nanometer scale based on protein-polymer assemblies as compartments with triggered activity that are able to function as mimics of natural organelles inside cells (Figure 1).[2] Such artificial orgenelles are generated by simultaneous insertion of biopores/membrane proteins inside the membrane of compartments, and encapsulation of active compounds (enzymes, proteins, mimics) inside. Biopores/channel proteins selectively control the exchange of substrates and products with the environment of nanocompartments, resulting in development of stimuli-responsive compartments, which preserve their architecture, while allowing specific *in situ* reactions. Upon up-take by cells, these artificial organelles preserve their integrity and start to function in the presence of the specific stimulus (pH, reductive conditions). Such artificial organelles open new avenues in various domains, as for example protein therapy or biosensing approaches.

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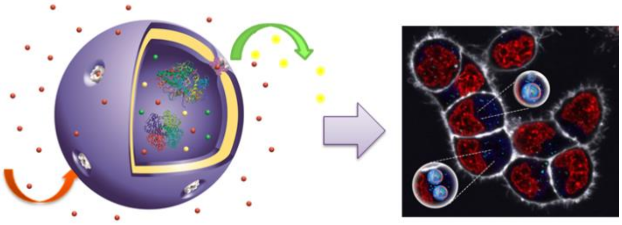

Figure 1. Concept of an artificial organelle with triggered activity inside cells based on encapsulation of a specific enzyme, and insertion in the membrane of the nanocompartment of a chemically engineered protein "gate".

New cross-linking method of halogenated butyl rubber nanocomposites

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Butyl rubber (IIR) posses broad range of industrial applications, including production of tires, inner tubes, gaskets, electrical insulators, shock absorbers, hoses, adhesives and sealants, rubberised fabrics, aircraft engine mounts, conveyor belts as well as pharmaceutical closures [1,2]. This can be attributed to its unique properties, such as low gas permeability, exceptional heat resistance and compression-set properties or good resistance to ozone and solar radiation action [2].

Butyl rubber is synthesized from isobutylene in solution polymerization process. Unfortunately, there are no double bonds available for cure. Wherefore a small amount of isoprene is added to the polymerization process in order to provide unsaturated bonds necessary for cure. Additionally, halogenation process of butyl rubber can be carried out to add cross-linking sites into polymer structure [3].

Numerous studies have been dedicated to the vulcanization issue of butyl rubber. Nanocomposites made of butyl rubber can be cross-linked with conventional sulfur based systems (in the presence of active accelerators), peroxides or phenolic resins [2- 5]. Notwithstanding, in order to improve efficiency of this process, it is essential to find out an alternative.

In our work we applied metal complexes in combination with triethanolamine as cross-linking systems [6]. It is likely that cross-linking reaction proceeds in accordance with Heck mechanism.

This work aimed to study the effects of new curing agents on cross-linking process of bromobutyl rubber (BIIR). Composites filled with montmorillonite or carbon black were prepared. The rheometrical properties of rubber compounds as well as cross-linking degree and mechanical properties of vulcanizates were tested. Additionally, composites were subjected to thermo-oxidative ageing process and afterwards ageing coefficient was determined.

It has been found that metal complexes are active cross-linking agents.

Obtained vulcanizates indicated high value of cross-linking degree and demonstrated good mechanical properties. Furthermore nanocomposites exhibited outstanding barrier performance as well as improved thermal properties.

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Graphene on SiO_2 under ultrahigh pressure

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Since the first isolation of graphene [1], silicon dioxide (SiO_2) has been one of the most used supporting substrate, due to its insulating properties and its easy integration in silicon based electronics. Interestingly enough, theoretical predictions still give controversial results on the binding mechanism of graphene on SiO_2; some works indicate strong chemisorption[2], other authors [3] suggest weak physisorption; finally, other works [4] suggest that both chemisorption and physisorption on SiO_2 are possible, depending on the surface cut.

Atomic Force Microscopy experiments on graphene placed on an amorphous SiO_2 surface shows a dramatic irreversioble change in graphene's height profile, after the application of high pressure (tens of GPa) to the system by means of a diamond tip. These finding seem to suggest that both chemisorption and physisorption of graphene are possible on the very same surface of SiO_2, with the transition triggered by the high pressure.

To clarify this rich scenario, we investigated the binding mechanism of graphene on different SiO2 surfaces by means of Density Functional Theory (DFT) calculations. We found that a stable configuration always exists in which graphene is physisorbed to the SiO_2 substrate, i.e. it is bound by weak dispersion forces at a distance of ~3Å. Furthermore, we found that, depending on the particular surface cut, several stable arrangements of C atoms exist on the SiO_2 surface, in which one or more C atoms are chemically bound to either the Si or the O atoms of the surface. Among these configurations, we focused on the ones retaining the honeycomb lattice, characteristic of freestanding graphene. With the aim of clarifying whether the application of high pressure could induce the transition from the weakly bound physisorbed graphene to the strongly interacting chemisorbed one, we run DFT calculations on coordinate paths connecting the chemisorbed and physisorbed configurations. Our calculations (Figure 1) show that the chemisorption and the physisorption are two possible energy minima in the configuration space, separated by a energy barrier and, more itnerestingly, by a pressure barrier of the order of 10-20 GPa, confirming the experimental findings.

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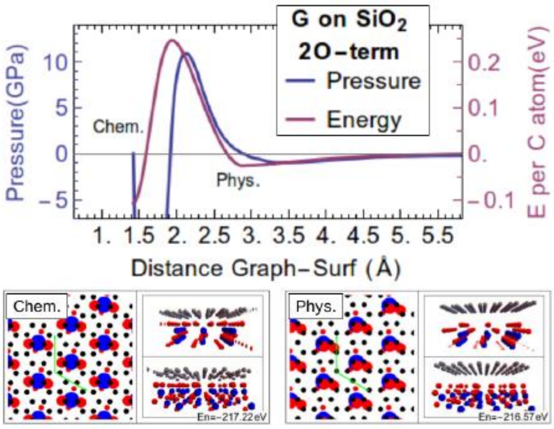

Figure 1. (Top) Pressure and energy barriers separating the chemisorbed configuration (bottom left) and the physisorbed one (bottom right) for graphene on a 2º terminated SiO_2 slab.

Polymer-SWCNT composites for recovering waste heat into electrical energy

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Singlewalled carbon nanotubes (SWCNTs), consisting of rolled graphene sheets with fullerene end caps, are not only used to incorporate the function of electrical conductivity into insulation polymers but also to create thermoelectric materials which are able to recover waste heat into electric energy. The thermoelectric (TE) effect (also called Seebeck effect) is evidenced as an electrical potential (voltage ΔU) induced by a temperature difference (ΔT) between the two sides of a material. High Seebeck coefficient, high electrical conductivity and low thermal conductivity are favourable for a high TE efficiency of a material. The advantages of polymer based thermoelectric materials are not only their cost efficiency, but also the ease of processing, flexibility, low density, and intrinsic low thermal conductivity.

SWCNTs of the type TUBALL^{TM} from OCSiAl were employed to construct an electrical conducting network in a polypropylene (PP) matrix by melt processing in a twin-screw compounder. For these SWCNTs a very low electrical percolation threshold of ~ 0.1 wt% was found [1]. The effect of SWCNT content on electrical conductivity and Seebeck coefficient (S) was studied. In addition, the addition of copper oxide (CuO) powder, a nontoxic compound with high S value, together with CNTs was shown to enhance the S of the composites [2]. Furthermore, the addition of an ionic liquid (IL) as processing additive during mixing improved the electrical conductivity of the composites and simultaneously increased S [3]. The maximum S value reached was 63.8 μV/K, resulting in a power factor of 0.26 $\mu W/(m \cdot K^2)$.

With the aim to demonstrate the applicability of melt mixing to fabricate thermoelectric generator (TEG), an easy and cheap route to switch p-type into n-type composites was developed since for an TEG both types are needed. At the investigated SWCNT concentrations (0.8 wt% and 2 wt%) and a fixed CuO content of 5 wt%, the polyethylene glycol (PEG) addition converted p-type composites (positive S value) into n-type (negative S). To construct the demonstrator, two composites were selected: p-type PP/SWCNT composite (with S up to 45 μV/K), and n-type composite (with S up to -56 μV/K) using PEG. The two prototypes with 4 and 49 thermocouples of these p- and n-type composites delivered output voltages of 21 mV and 110 mV, respectively, at a temperature gradient of 70 K (Fig. 1).

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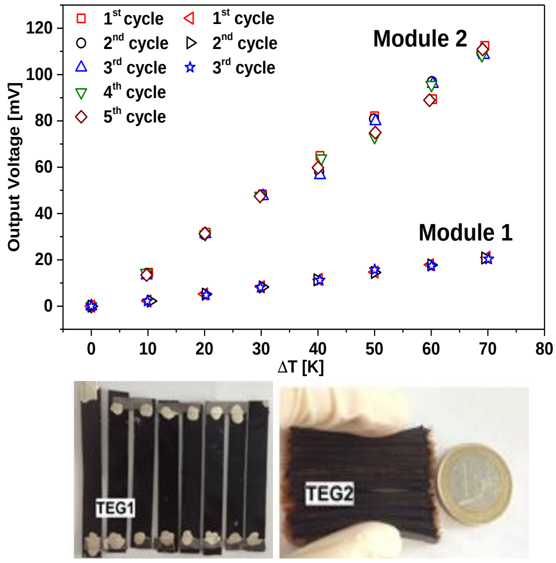

Figure 1. Thermo-electric output voltage versus ΔT for two prototype thermoelectric generators (TEG1 and TEG2) [4]

Millisecond annealing for the nanoscale

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Semiconductor structures with nanometer dimensions become more and more important in microelectronics and other new emerging technologies. However, the transition from bulk materials to nanostructures often requires significant changes in the process technology, including the change from equilibrium to non-equilibrium processes. In this work, we investigate the formation of nanodots and the modification of nanowires by millisecond flash lamp annealing [1].

In detail, we focus on two specific topics: (i) the formation of InAs nanocrystals in a thin Si layer at laterally defined positions with the help of masked ion beam implantation and flash lamp annealing, and (ii) the high-level doping of Si and Ge nanowires by ion implantation and flash lamp annealing.

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Biomimetic Synthesis of Polyaniline Catalyzed by Hematine Supported on Graphitic Carbon Nitride

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Polyaniline is a versatile intrinsic conductive polymer easy to synthesize through several chemical and electrochemical methods. However, those require further processing steps to obtain a polymer for practical applications in such fields as nanocapacitors, biosensors and many others (Fig. 1A). Enzymatic synthesis have been merge as interesting alternative to produce polyaniline and other intrinsically conductive polymers, where the only subproduct of the reaction is water, but the main drawbacks of this method is that the peroxidases used as catalyst usually lose their actithe pH acid needed to carry out [1]. Hematin is natural compound that biomimicry the activity of the poxidases and has been used for our group and others to catalyst the synthesis of aniline. To the difference of the proxidases, hematin catalyst the synthesis of polyaniline at pH acid without suffer inactivation during the polymerization reaction [2].

In recent years, the two-dimensional materials are aroused intense scientific development due to its exceptional properties. Graphene is one of the most prominent candidates to revolutionize the industry. However other alternatives such as Carbon Graphite Nitrides have proven to be structured with a high potential in the area of photocatalysis, its application have of metallic colloids, organic catalysis and so on [3].

The so-called g-C_3N_4 is the most stable polymorphic analog of carbon nitride and has been the subject of great attention in the last 5-6 years (Fig. 1B). Here, we present the obtained result of the solar-thermal synthesis of g-C_3N_4 to be used as support of hematin that works like biomimetic peroxidase in the catalyst of aniline, which materials could leads to obtaining a hybrid with potential characteristics for the The synthesis of XRD g-C_3N_4 by solvothermal treatment was analyzed using X-ray diffractometry, UV-vis, FTIR, Raman, and XPS spectroscopies. The obtained results together with SEM, HR-TEM and AFM microscopies and thermal characterization are indicative of the successful synthesis of this material (Fig. 2B).

The changes in absorption bands in the UV-vis spectrum associated to the hematin after be deposited g-C_3N_4 layers has been explained as a complex in-teractions π-π* between this compound and the g-C_3N_4 layers[4]. Finally,we found that the hematin was a high efficient catalyst in the polymerization of aniline as is shown in the Tem images, FTIR and UV-vis spectra (Fig. 2C).

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Figures

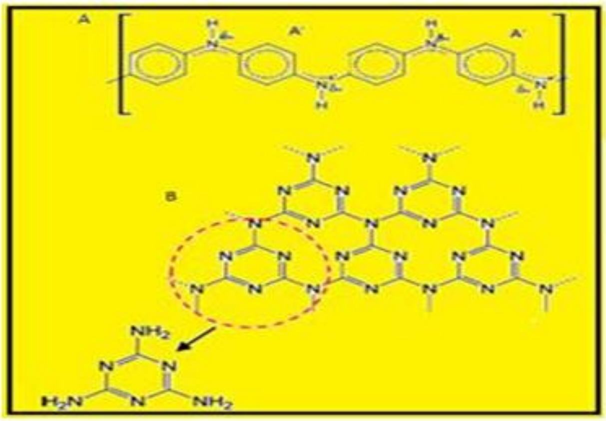

Figure 1. Schemes of the chemical structures of (A) polyaniline and (B) tris-s-triazine of g-C_3N_4

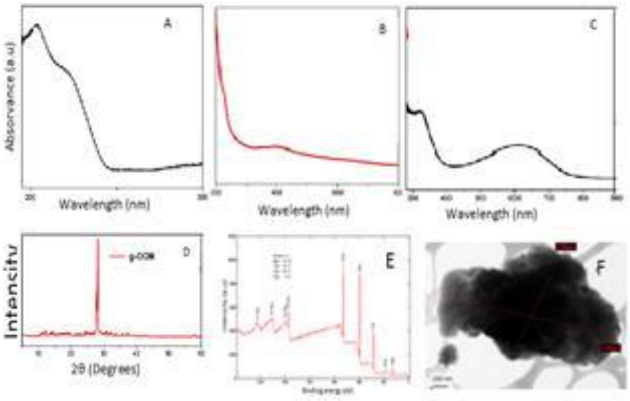

Figure 2. UV-vis spectra of (A) g-C_3N_4, (B) g-C_3N_4 hematin, (C) g-C_3N_4 hematin-Polyanilina, (E) XRD of g-C_3N_4 and XPS of g-C_3N_4

Hybrid Materials from Sculptured Thin Films and Applications

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Coherently ordered nanostructures establish a new class of surfaces, created by a regular arrangement of congruent, three-dimensional-shaped nanostructures. Shape, size, and relative position of the nanostructures allow nearly limitless combinations. Size and relative position can be varied from nanometer to micrometer regions. This presentation focusses on the extremely anisotropic optical properties of highly-ordered three-dimensional nanotopographies known as sculptured columnar thin films (SCTFs). We discuss tailored deposition of single and heterostructure [1] SCTFs and core-shell structures [2,3] using ion-beam and electron-beam assisted glancing angle and plasma-assisted atomic layer deposition techniques from a large variety of materials [1-5]. We will show and discuss how these materials have enabled the creation of new sensing and separation techniques for molecular interactions at the surfaces and interfaces [3], the invention of anisotropy contrast optical microscopy and imaging chromatography [4]. We will demonstrate exemplary applications to imaging molecular interactions and living cells [5], and fluidic separations at the nanoscales [4].

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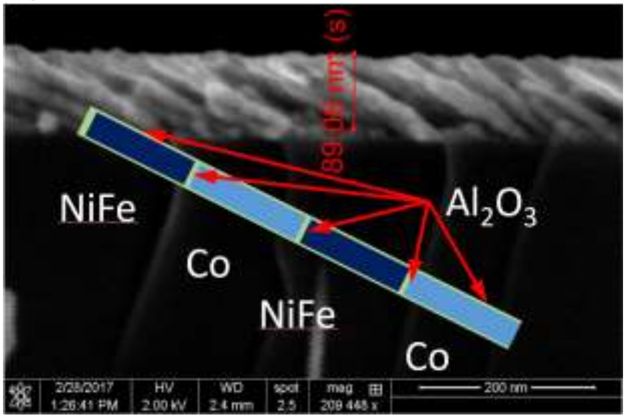

Figure 1. Slanted Columnar Heterostructure Thin Film (SCHTF) with 1dimensional junctions for tailored magnetism [1].

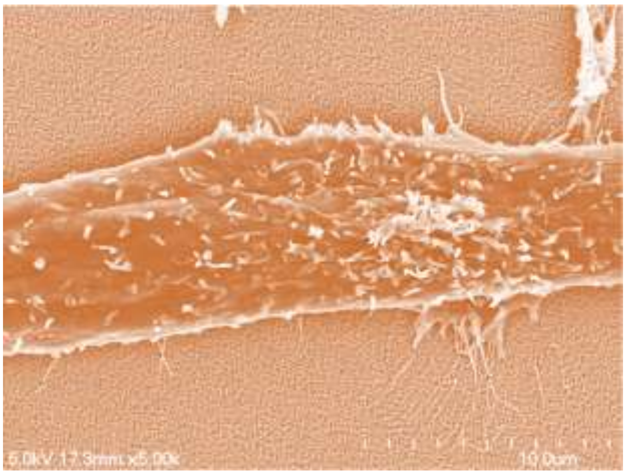

Figure 2. Stimulated cell-substrate interactions of NIH/3T3 mouse fibroblasts on titanium STFs. [5]

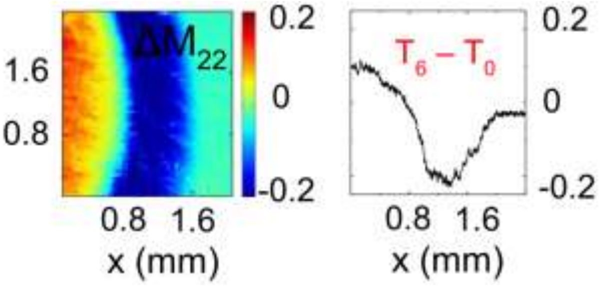

Figure 3. Anisotropy contrast of chromatographic separation of lipophylic dyes within SiO2-SCTF [4].

Tailored nanoporous SiO_2 thin films for antireflection coatings

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Nanoporous materials are essential in numerous applications ranging from membrane technology for e.g. separation und purification, to semiconducting and photonic industry, as low-k and low-n materials. The established methods for the synthesis of nanoporous layers encounter their limits especially if conformal coatings on high aspect ratio surfaces are required. The precise control of the porosity is also challenging. We developed a new procedure to deposit nanoporous silica (SiO_2) thin films by mixing ALD Al_2O_3 and SiO_2 in an Å-scale and subsequently removing the Al_2O_3. The composition of the films can be varied by simply adjusting the number of ALD cycles for Al_2O_3 and for SiO_2 during the process. The alumina is selectively removed in H_3PO_4 solution and the formation of nanoporous SiO_2 films is observed. The porosity and subsequently, the refractive index of the nanoporous SiO_2 films can be precisely tailored by the initial composition of the films. The porosity increases with increasing Al_2O_3 content of the ALD coating.

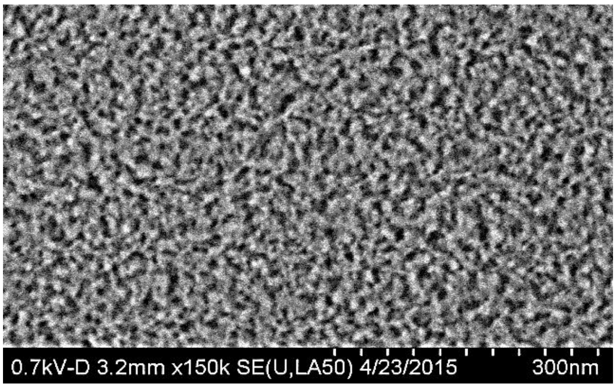

Figure 1. Scanning electron micrograph of a highly nanoporous SiO_2 thin film with a porosity of ca. 70%

Figure 1 shows a scanning electron microscopy image of nanoporous SiO_2 thin film. The porosity of this film is ca. 70% with a refractive index of approximately 1.13 at 633 nm wavelength. These coatings are highly interesting for antireflection applications. Single layer antireflection coatings have been demonstrated by simultaneously coating front and backside of quartz substrates. The film thickness of the coating determines the wavelength of the minimum reflectance.

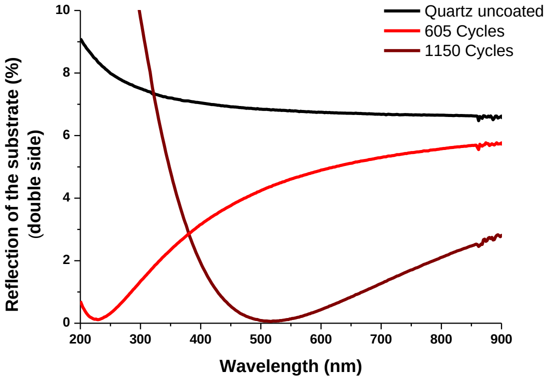

Figure 2. Reflectance spectra of double side coated quartz substrates. The total reflectance of the uncoated substrate is approximately 7%.

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Nitrogen and Boron Doping Effects in Carbon Nanospheres

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Abstract

Carbon nanospheres (CSs) are attracting more attention worldwide due to their excellent performance in various fields such as drug delivery, heterogeneous catalysis and encapsulation of support materials. Carbon atoms in CSs can be replaced with other atoms in the carbon matrix which alters the physical and chemical properties of the spheres. Typical elements that are used as dopants are N, B, S and P. These heteroatom dopants in carbon materials provide improved and controllable electronic features and rich surface chemistry, thus play an increasingly important role in nanocarbon-enabled advanced functional materials, e.g. sensors[1], energy storage materials[2] and heterogeneous catalysts[3]. Heteroatom doped CSs can be solid, hollow or core-shell in morphology. Different methods have been used to synthesize CSs, and some require a catalyst, a soft or hard template. Of the available methods for the synthesis of solid and hollow CSs, the chemical vapour deposition (CVD) route seems the most viable due to its simplicity and low-temperature of operation; and for the fabrication of hollow CSs it is better than hard templating routes, since the extra steps and use of harsh etching agents (typically HF) to remove hard templates make processing tedious. Herein we report a simple method for the growth of nitrogen doped carbon spheres (N-CSs) and boron-doped hollow carbon spheres (B-HCSs) without using a catalyst or a template. N-CSs were synthesized via a CVD method at 900 °C using C_2H_2 as the carbon precursor and CH_3CN as a C and N source. For the B-HCSs growth, a similar set-up to N-CSs synthesis was used, and C_2H_2 was used as the carbon precursor and $B(OCH_3)_3$ as a C and B source. The N-CSs and B-HCSs were synthesized using vertical furnace and the properties of the produced materials were compared to CSs synthesized using C_2H_2 as a C source. The morphology, structural features and the composition of the CSs, N-CSs and B-HCSs were ascertained by TEM, HAADF-STEM, TGA and XPS. Fig. 1 shows the TEM image of B-HCSs. Compared to TEM images of CSs and N-CSs (not shown here), which appeared solid, the morphology of the B-HCSs was hollow while some had core-shell morphology. TGA analysis confirmed the presence of the B_2O_3 (25-35%) in the crude product and this B_2O_3 could be removed by boiling water. HAADF-STEM (not shown here) analysis confirmed the presence of B_2O_3 in the centre of the core-shell boron doped carbon spheres. Using XPS analysis, the N content in the N-CSs was found to be 3.10%. The level of boron content in the B-HCSs was found to be 3.92 % (mainly B_2O_3). The final residual B found in B-HCSs was associated with B doping. The B_2O_3 acted as a template for the formation of the B-HCS structures and a mechanism for the B-HCS formation is proposed.

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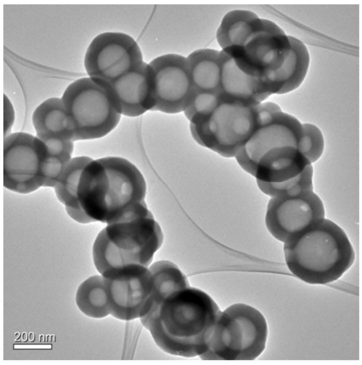

Figure 1. TEM image of B-HCSs

Multifunctional Water Soluble Carbon Nano Onions from Flaxseed Oil for Visible Light Induced Photocatalytic Applications and Label Free Detection of Al(III) Ions

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CNOs are a new group of ultra-small carbon nano structures with unique physiochemical properties due to pronounced quantum confinement and edge effects and a one of the fastest moving and most exciting nanotechnologies research concern.[1,2] Onion-like carbon nanoparticles (CNOs) were synthesized via traditional pyrolysis of flaxseed oil. Oxidative treatment of as-synthesized carbon soot introduced numerous carboxyl (-COOH) functionalities, rendering them hydrophilic and stable in aqueous phase. The water-soluble onion-like carbon nanoparticles (wsCNOs) were 4-8 nm in size and exhibited stable green photoluminescence (PL) emission. CNOs were explored as efficient photocatalysts for the degradation of methylene blue (MB) as model organic pollutant dye under visible light irradiation. The wsCNOs exhibited photocatalytic efficiency ~9 times higher than CNOs for MB degradation. Enhanced photocatalytic efficiency of wsCNOs was attributed to their surface functionalities and nanostructure. The unique morphology (concentric nanographene shells) with considerable surface defects, increased the physisorption of MB on the wsCNOs surface and significantly enhanced the photocatalytic efficiency of wsCNOs. Furthermore, the wsCNOs enabled specific detection of Al(III), even with interference from high concentrations of other metal ions, with a detection limit of 0.77 µM, which compares favorably to other reported fluorescent probe. Altogether, the wsCNOs showed a significantly enhanced photocatalytic activity and were used as highly selective fluorescent probes for Al(III) ion detection, suggesting a potential use in environmental wastewater treatment. In addition, Flaxseed oil soot can be an ideal building block and open up new window for the fabrication of composite material for multifunctional applications.[2,3]

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Figure

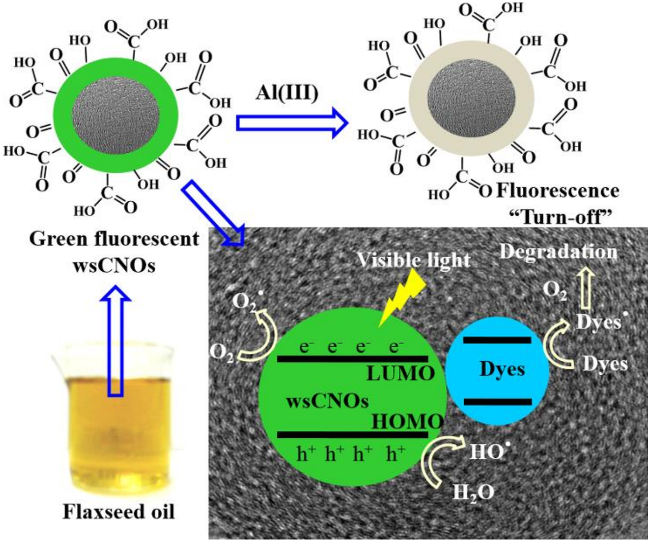

Figure 1. A schematic representation for the synthesis and multifunctional application of water soluble green fluorescent carbon nano onions.

Efficient Hydrogen Production by Tailoring Electrocatalysts with Fast Water Dissociation Kinetics

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Large scale and sustainable production of hydrogen from water using the efficient and cost-effective electrocatalytic/photocatalytic/photoelectrocatalytic water splitting devices, e.g., water-alkali electrolyzers, is greatly promising for the future hydrogen economy.[1] To this end, efficient, durable, and low-cost electrocatalysts are required to reduce the kinetic overpotentials of hydrogen evolution reaction (HER).[2] Noble metal platinum (Pt) has been recognized as the most active and robust HER electrocatalyst with a near-zero onset overpotential and a high anodic current density. Unfortunately, the large-scale employment of Pt catalysts for hydrogen production is severely limited by its scarcity and high cost.

For the HER in an alkaline solution, the kinetic process involves two steps: the prior water dissociation (Volmer step) and the subsequent combination of the adsorbed hydrogen (H*) into molecular hydrogen.[3] Thus, once an electrocatalyst facilitates the initial water dissociation step on the surface, the HER performance will be improved. In this regard, we developed and design the novel electrocatalysts through engineering active sites for the water dissociation.[4,5] For example, we demonstrate a novel out-diffusion strategy for synthesizing $MoNi_4$ electrocatalysts, which can efficiently speed up the sluggish the Volmer step of the HER process in alkaline solution.[6] The computational and experimental results reveal the fact that the kinetic energy barrier of the initial Volmer step is substantially reduced on the $MoNi_4$ electrocatalysts. The as-constructed $MoNi_4$ electrocatalysts supported by MoO_2 cuboids exhibited an excellent electrocatalytic HER activity in 1 M KOH aqueous solution with an extremely low overpotential of ~15 mV at a current density of 10 mA cm^{-2} and a low Tafel slope of 30 mV $decade^{-1}$, which are highly comparable to the results for the Pt and superior to those for state-of-the-art Pt-free electrocatalysts. Benefiting from its scalable preparation and excellent stability, the developed $MoNi_4$ electrocatalyst is highly promising for practical water-alkali electrolyzer.

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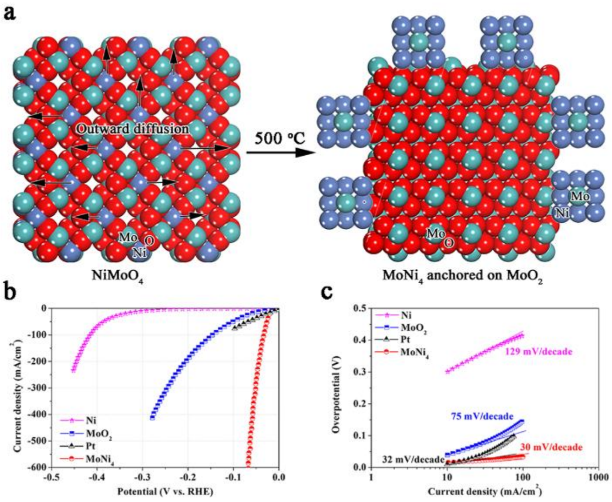

Figure 1. a) The synthetic scheme of the $MoNi_4$ electrocatalyst supported by the MoO_2 cuboids on nickel foam. b) The polarization curves and (c) Tafel plots of the electrocatalysts.

TNT2017 Orals – Students contributions

Bypassing the rumen using lipid nanoparticles

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Feed digestion in ruminant animals largely rely on rumen microbial fermentation. The microbiota of the rumen extensively degrades dietary protein, the resulting products being incorporated into their own microbial proteins, while lipids pass through relatively unscathed. Since microbial protein digested in the small intestine is not sufficient to meet the amino acids requirement of high producing animals, an effective protection of feed N from rumen fermentation is needed. In the present study, we propose a new approach that takes advantage of nanotechnology to bypass the microbial fermentation in the rumen, but also to increase the absorption of the nutrients into the bloodstream, relying on lipid nanoparticles (NPs).

A wide variety of different formulations were proposed and tested, consisting of solid lipid nanoparticles (SLN), nanostructured lipid carriers (NLC) and multiple lipid nanoparticles (MLN). All these formulations were characterized in terms of size, polydispersity index and zeta potential and their stability in rumen inoculum assessed.

Results showed that only SLN formulations composed of stearic acid and arachidic acid could resist digestion in the rumen inoculum, maintaining their size range of 300-500 nm after incubation and with a highly negative surface charge of around -35 mV. Transmission electron microscopy images confirmed that both SLN could resist digestion and maintain both their size and spherical morphology.

The NPs were loaded with lysine and an adequate quantification method, based on high performance liquid chromatography (HPLC) with fluorescence detection of dansylated derivatives, was developed. Using this method, the encapsulation efficiency of the formulations was determined, rendering values of up-to 40%.

To conclude, this preliminary study showed that SLN could be synthesized, with adequate physical properties, and with the ability to resist digestion in the rumen, retaining their size, zeta potential and morphology. They were also capable of being loaded with a highly hydrophilic molecule with reasonable efficiency. The proposed formulations are, therefore, promising candidates for future rumen-bypass applications in ruminant nutrition and may help to surpass the current limitations of the existing technologies and products.

Acknowledgments:

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Figures

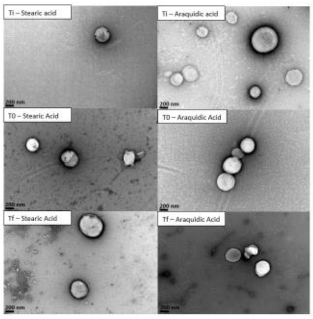

Figure 1. Transmission electron micrographs of NPs after synthesis (Ti), after contact with rumen inoculum (T0) and after 24h incubation at 39 °C in rumen inoculum (Tf).

Layer-By-Layer multilayer assembly of Graphene oxide with Keggin-type Polyoxometalates for electrocatalysis of Chloroform

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Multilayer assemblies of the Keggin-type POM [$H_4SiMo_{12}O_{40}$] and Graphene Oxide (GO) have been immobilized onto glassy carbon electrode surfaces via the layer-by-layer (LBL) technique employing the PEI as the cationic layer. Resulting thin films were characterized by different electrochemical and surface techniques. The redox behavior of both the immobilized POM and the Graphene oxide are observed. The resulting films were found to be highly conductive through the employment of AC impedance. It exhibited significant electrocatalytic properties towards the reduction of chloroform in water (as shown figure 1).

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Figures

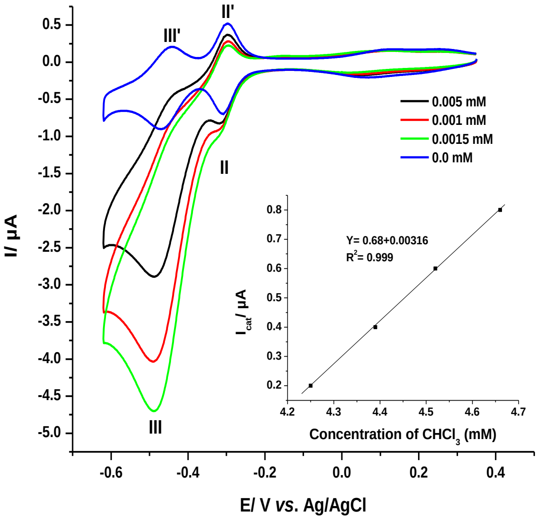

Figure 1. Cyclic voltammogram of the multilayer assembly of GO/PEI/$H_4[SiMo_{12}O_{40}]$ (outer anionic layer of POM) in buffer solution pH 7.0, before (0.00mM) and after addition of chloroform (0.002mM , 0.005mM, 0.001mM) at a scan rate of 10 mVs^{-1}. The inset shows the relationship between the catalytic current (I_{cat}) and the chloroform concentration for the Mo-III wave.

Multiplexed Synaptic Modulation and Memory in Ionic Film-coated Si Nanowire Transistors

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The brain has remarkable memory and learning ability using parallel information processing in multiple synapses.[1] By mimicking the brain functionality, artificial synapses have been established using memristors[2] and transistors[3] based on synaptic plasticity of ionic or memristive film. However, to realize the feasible learning and memory for neurocomputing is still in challenge because of the low compatibility of the memristive devices with conventional Si-based CMOS system and an unintuitive memory process using the timing between pre- and post-synaptic signals.[4] Here, we report synaptic Si nanowire transistors covered with ion-doped silicate film. A planar top gate can simultaneously modulate the conductivity of multiple post-synaptic nanowires through the film that would be able to realize multiplexed neurotransmission in the brain. The synaptic transistor acts as a random access memory (RAM) cell due to the ionic polarization of doped metal ions in the film depending on amplitude and frequency of pulses applied on the gate. Therefore, short term potentiation (STP) is configured by the transfer characteristics of a transistor. In addition, synaptic learning has been appeared after rehearsed training, so that the post synaptic current reaches the same current level faster than before training. This study has achieved a breakthrough in the convenient interconnection between neuromorphic devices and CMOS system with tunable memory mimicking the process of human brain.

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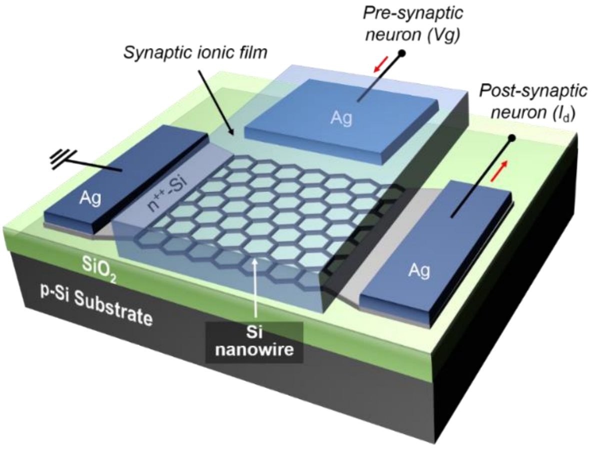

Figure 1. Schematic diagram of the synaptic Si nanowire field effect transistors (FETs)

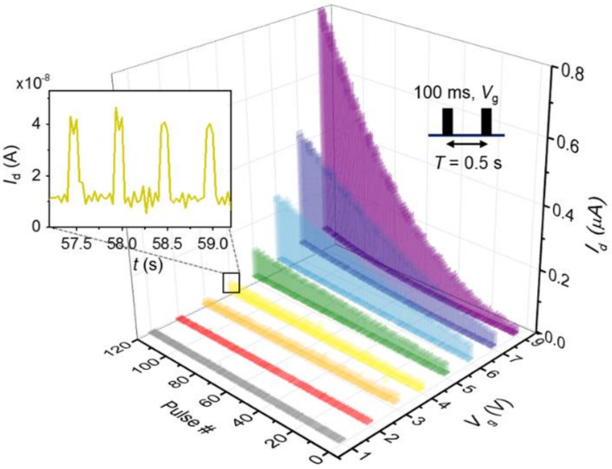

Figure 2. Synaptic plasticity depending on the gate bias

Toward integrated detection and graphene-based removal of contaminants in a lab-on-a-chip platform

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In this work a miniaturized microfluidic platform for the simultaneous detection and removal of polybrominated diphenyl ethers (PBDEs) is developed. This device consists of a polydimethylsiloxane (PDMS) microfluidic chip for an immunoreaction step, a PDMS chip with an integrated screen-printed electrode (SPCE) for detection and a PDMS-reduced graphene oxide (rGO) chip for physical adsorption and subsequent removal of PBDE residues. The detection was based on competitive immunoassay (PBDE vs. HRP-PBDE) followed by the monitoring of enzymatic oxidation of o-aminophenol (o-AP) using square wave anodic stripping voltammetry (SW-ASV). PBDE was detected with the limit of detection similar to that obtained with a commercial colorimetric test (0.018 ppb), but with the advantage of using lower reagent volumes and a reduced analysis time. The use of microfluidic chips also provides improved linearity and a better reproducibility in comparison to those obtained with batch-based measurements using screen-printed electrodes. In order to design a detection system suitable for hazardous compounds such as PBDEs, a reduced graphene oxide–PDMS composite was developed and optimized to obtain increased adsorption (based on both the hydrophobicity and π–π stacking between rGO and PBDE molecules) compared to those of non-modified PDMS. To the best of our knowledge, this is the first demonstration of electrochemical detection of flame retardants and a novel application of the rGO-PDMS composite in a biosensing system. This system can be easily adjusted to detect any analyte using the appropriate immunoassay and it supports operation in complex matrices such as seawater.

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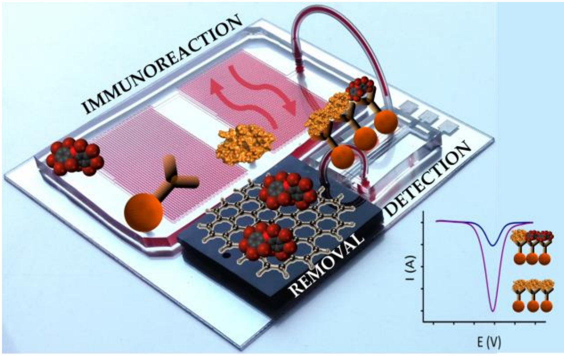

Figure 1. Lab-on-a-chip platform for electrochemical detection and graphene-based removal of polybrominated diphenyl ether (PBDE).

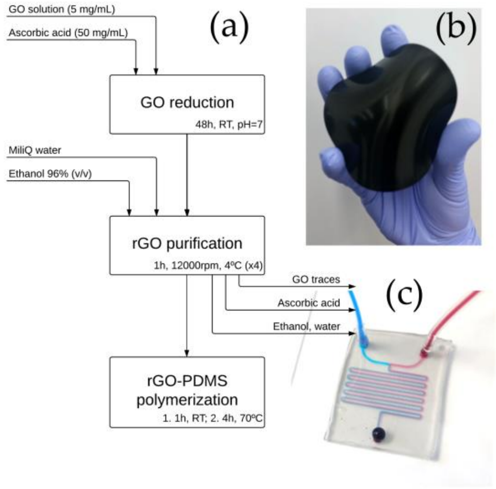

Figure 2. rGO-PDMS composite (a) fabrication process, (b) a solid piece or rGO-PDMS, (c) rGO-PDMS-glass microfluidic chip

Tailoring Fermi's velocity in topological insulators by an electric field

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Combined with band-engineering techniques, topological insulators could dramatically boost and reshape the current state-of-the-art in electronics. Parameters such as the Fermi velocity are of great relevance to this issue, and their flexible manipulation would allow to largely broaden the spectrum of possibilities. So far, however, changes in the Fermi velocity require very cumbersome setups, making them rather unpractical for real applications [1-3].

In this work, I will present a theoretical mechanism that enables to tailor Fermi's velocity avoiding both structural and configurational alterations. Despite of being a theoretical prediction, it can be readily achieved experimentally. The system at hand is a double-gated band-inverted junction. Here, a heterostructure is built by growing a band-inverted semiconductor, followed by a conventional semiconductor, thus forming a sharp junction (attainable by molecular beam epitaxy techniques) where the aforementioned edge states take place. A two-band Dirac model has proven to be the most suited one for describing the electronic states of these systems [4-5]. This model allows us to consider a uniform electric field (achievable by means of front- and back-gates) and is exactly solvable, as we have shown [6]. However, one can gain further intuition by applying some reasonable approximations that lead to our main result: Fermi's velocity can be substantially lowered, becoming a tunable parameter. This result matches the exact calculations in the experimentally feasible range of fields considered for the approximation. Hand-waving arguments capture the essential physics and are summarized in Figure 1.

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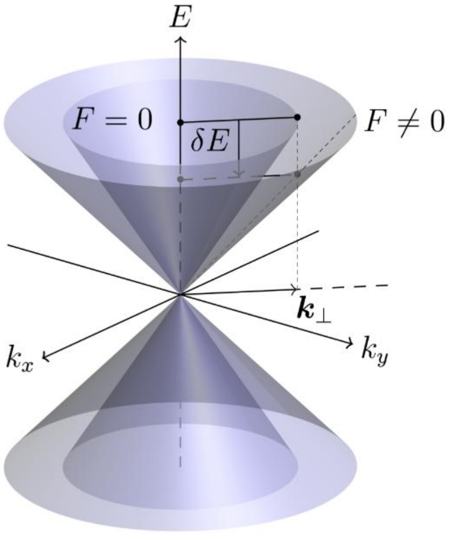

Figure 1. Dirac cones of the edge states at zero and finite electric field F, applied perpendicular to the interface. By adiabatically switching on the electric field, there is a decrease of the electron energy of magnitude δE. Since the interface momentum $\boldsymbol{k}_\perp$ is conserved, the cone must then widen, thus leading to an effective reduction of Fermi's velocity.

Performance enhancement of carbon nanotube FETs via polymer-based doping control

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Abstract

The direct synthesis of polymers like sodium 4-styrenesulfonate inside the channel of carbon nanotube (CNT) based field-effect transistors (FETs) strongly improves the device performance. Starting with monomeric compounds, the FET-channel was *in-situ* passivated, using the self-initiated photografting and photopolymerization process [1]. An exemplary CNTFET as well as the polymer integration procedure is elucidated in Figure 1. Upon formation of the polymer matrix, we report increased drain currents as well as on/off current ratios, an improved device-to-device consistency, and lower variability in the threshold voltage. The change of the electrical transfer characteristics of the CNTFETs upon polymer passivation as well as a statistical evaluation of the on conductance and on/off current ratios for more than 60 devices are illustrated in Figure 2. Annealing in vacuum was shown to further improve the device performance and induces an ambipolar transport behavior due to a removal of water molecules in vicinity of the CNTs. Additionally the devices showed a long-term stability upon storage under ambient environment [2]. We present a systematic study based on different polymer integration procedures enabling to adjust the properties of CNTFETs. Those procedures elucidate improvements in essential figures of merit of the FETs by several orders of magnitude especially for wet-processed CNTFETs. We discuss the underling mechanisms based on electrical, structural and simulation studies.

This channel engineering approach opens new possibilities to tune CNTFETs key parameters that facilitate a wide application covering especially high frequency CNTFET devices and also thin film CNT transistors for flexible electronics.

Figures

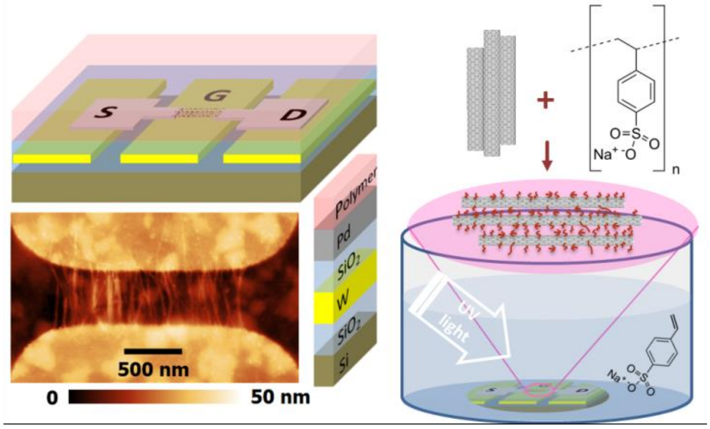

Figure 1. Schematic illustration of one CNTFET (left) and of the polymer integration procedure (right) [2]

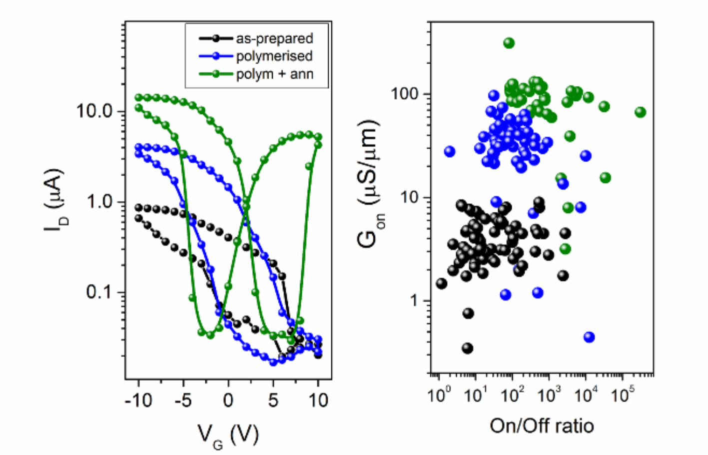

Figure 2. Electrical transfer characteristics of one CNTFET (left) and a statistical analysis of the on conductance and on/off current ratios of over 60 devices (right) [2]

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Structural Analysis of Plasma Exfoliated Graphene Nanoplatelets (GNPs) for the Development of Nano-Cementitious Composites

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Abstract

Graphene and its derivatives, especially graphene oxide (GO), gained much attention for its use in cementitious matrix to improve mechanical properties of cementitious composite. GO is widely synthesized by chemical surface modification using modified Hummer's method in recent years. The chemical surface modification techniques generally use harsh chemicals and acid which may degrade the structural and mechanical properties of graphene. Plasma exfoliation is a new sophisticated technologically enhanced method for graphene synthesis and functionalization without using any harsh chemicals. Plasma exfoliated graphene nanoplatelets (GNPs) functionalized with -O_2, -NH_2 and -COOH chemical groups were dispersed into the cement matrix for the development of nano-cementitious composite. The dispersion and interfacial interaction of GNPs with cement matrix entirely depends upon its structural and morphological characteristics. Therefore, these GNPs were analyzed for structural, morphological, surface functionality, chemical composition and disorder in crystal structure by using various characterization techniques such as HR-TEM, SEM, AFM, XRD, FTIR and RAMAN before harnessing them into the cement matrix. From the characterization data these GNPs seems promising candidate for the development of nano-cementitious composite due to its well defined honeycombed lattice structure with interlayer spacing of 0.20 nm (Fig.1), high aspect ratio, high surface energy due to I_D/I_G ratio in between 0.05 and 0.70 (Fig.2) and well dispersion capabilities in the aqueous solution.

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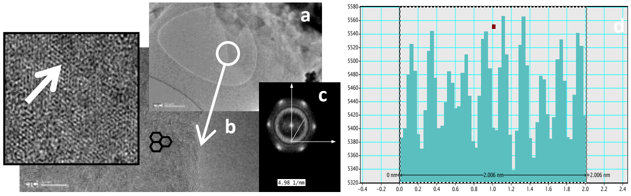

Figure 1. HR-TEM image of GNPs (a) single layered G-O2 on Cu grid (b) HR-TEM of the area spotted with white circle in fig.1a (c) FFT of G-O2 for analysis of spacing between lattice planes and (d) intensity profile taken along the white arrow shown in top left inset Fig.1b.

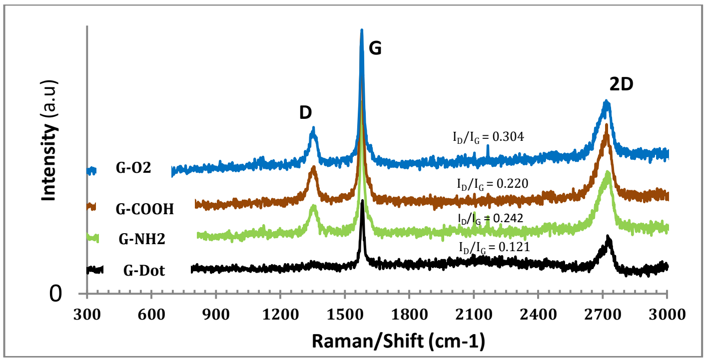

Figure 2.
Combined RAMAN spectrums of G-Dot and G-Fnt. indicating ID/IG ratios of GNPs in between pure graphite (0.05) and GO (0.70) [1]

Graphene mechanics: defects, buckling and domain growth

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We have developed a new semi-empirical potential for graphene [1], using DFT calculations for determining the various parameters, which for the first time includes a term for out-of-plane deformations. We have demonstrated the usefulness of this potential in studies of different kind of intrinsic defects (Stone-Wales defect, separating dislocations and grain boundaries). Our simulations show that the stress caused by these defects can be relieved by buckling, which extends to hundreds of nanometers. A detailed study of the formation energies of defects surprisingly revealed that the value for the formation energy depends on the type of boundary conditions [2]. Therefore it is necessary to specify the boundary conditions for the energy of the lattice defects in the buckled two-dimensional crystals to be uniquely defined. We have also theoretically described that the vibrational density of states (VDOS) can be used in probing the crystallinity of graphene samples [3]. The novel potential can be effectively combined with interlayer interaction, allowing the simulation of bilayer graphene and study the effect of twist angle on the structure and buckling [4]. Recently, we have described the universal shape behavior of a graphene gas bubble irrespective of its size. We show that for small gas bubbles (~10 nm), the vdW pressure is in the order of 1 GPa [5].

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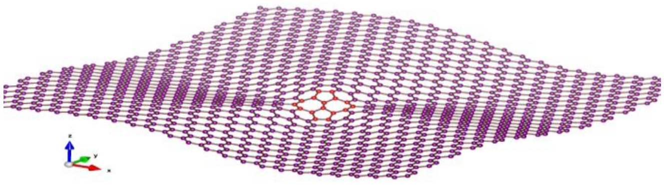

Figure 1. Buckled graphene with a Stone-Wales defect.

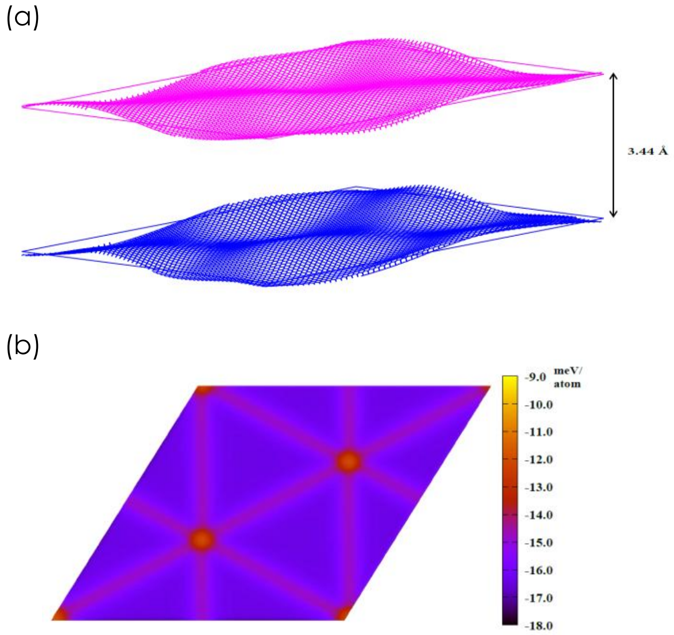

Figure 2. (a) Buckling in twisted bilayer graphene. (b) Energy distribution in twisted bilayer graphene and formation of vortices.

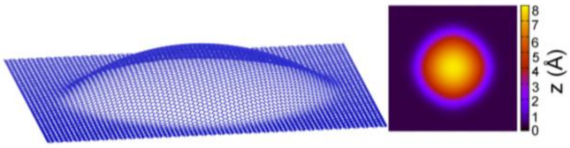

Figure 3. Structure of a graphene nanobubble. For small gas bubbles (~10 nm), the vdW pressure is in the order of 1 GPa.

Innovative Patterning Method for Modifying few-layer MoS_2 Device Geometries

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Mono-Layer and few-layer Tansition Metal Dichalcogenides (TMDCs) have attracted great interest since the discovery of graphene due to their oustanding properties[1-3]. Semiconducting 2D Molybdenum Disulfide (MoS_2) is considered a good candidate for opto-electronic applications due to its remarkable electrical and optical properties. However when mechanically exfoliated, these properties strongly depend on the geometry and number of layers present in the flake. In general, these properties cannot be modified once a device is fabricated out of an exfoliated flake. In this work we present a novel nano-patterning method for 2D material based devices, Pulsed eBeam Gas Assited Patterning (PEBGAP), that allows us to fine tune their properties once the device fabrication steps have been completed. This post-processing technique allows us to modify the channel geometry or thickness of MoS_2 FETs.

PEBGAP post-processing technique is based on using a scanning electron microscope equiped with a gas injection system, and employing XeF_2 as an etching agent. The etchant gas enters the chamber through a small nozzle situated in close proximity to the desired device, adsorbing locally on the substrate. The focused electron beam is then scanned and pulsed over the device to etch away the desired geometry onto the MoS2 flake.

Field effect devices were fabricated from mechanically exfoliated few-layer MoS_2 flakes via optical beam lithography followed by a metal evaporation and lift-off process to define the gate-contact structures. The devices were characterised employing µ-Raman mapping spectroscopy, transport measurements and AFM/SEM microscopy. Afterwards, PEBGAP was utilized to alter device geometries and performance.

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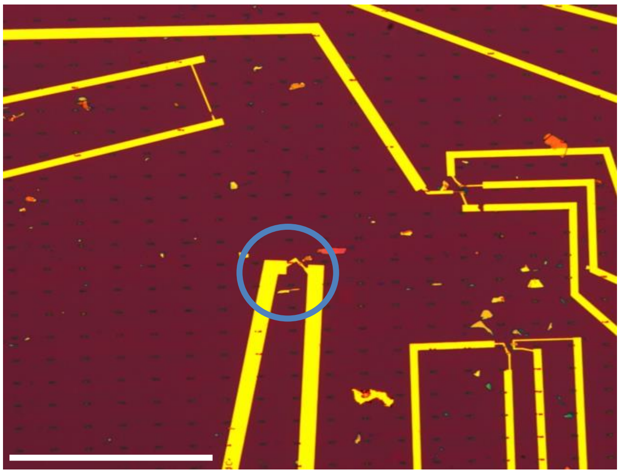

Figure 1. Optical image of a fabricated device. Blue circle indicates the chosen device to be patterned. Scale bar is 500 µm.

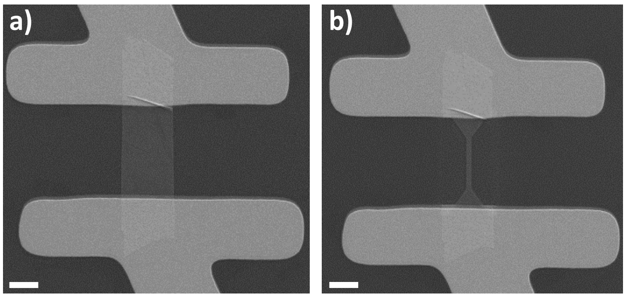

Figure 2. a) SEM image of the MoS_2 device circled in figure 1 before the PEBGAP patterning. **b)** SEM image after the XeF_2 PEBGAP pattern showing a narrowing of 500 nm. Scales bar in a) and b) are 1 µm

Ligand-free nanoparticles made by scalable laser synthesis for catalysis applications

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After decades of intensive research nanomaterials are widely implemented as functional elements on surfaces, into volumes and as nanohybrids, with a wide spectrum of applications such as catalysis and biomedicine. However, integration of the "nanofunction" into products is still limited due to drawbacks of gas phase and chemical synthesis methods. Ligands and stabilizers have to be removed by calcination and additives may cause catalysts poisoning. The quantitative removal of the ligands is very challenging and accompanied by unwanted side effects like particle aggregation and contamination causing deactivation of the building blocks' surface.

Pulsed Laser Ablation in Liquids (PLAL) makes it possible to fabricate ligand-free nanoparticles with high purities [1] and controlled size distribution [2] for a variety of materials (e.g. Au, Pt, Ni, alloys...). The naked nanoparticles have shown to better fit to kinetics expected by theoreticians, in particular at high conversion rates [1]. Hence, maybe purity is convenient for catalysis and nanoparticle application research, providing textbook-like reference materials.

Related to chemical energy conversion application, deposition of naked nanoparticles on inorganic and carbon supports creates heterogeneous catalysts with 100% cumulative yield and with mass loading up to 60% adjustable [3]. No calcination or pre-reaction activation is required since no chemical precursors or excess of reactants are employed which often have to be removed after conventional nanoparticle synthesis. Furthermore, recent findings indicate that the process stability of the catalyst during oxidative conversion at elevated temperature is increased during heterogeneous (supported colloids) catalysis [4].

The productivity of the laser-based nanoparticle production method is limited by different entities such as laser-induced cavitation bubbles [5], which contain the generated nanoparticles, and so-called persistent bubbles [6]. We could achieve good reproducibility and a linear up-scaling of nanoparticle generation by applying a continuous flow and using a high-power picosecond laser system consisting of a 500W ps-laser source and a laser scanner with scanning speeds of up to 500m/s. Nanoparticle outputs up to the gram/hour regime were obtained in this way making this method a versatile alternative for rapid prototyping of heterogeneous catalysts [5].

Overall, this talk is intended to give the audience an insight into the principles of the laser-based nanoparticle production process, the immobilization of the naked nanoparticles on particulate supports as well as the utilization of the nanoparticles in homogenous and heterogeneous catalysis.

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Optimizing geometric factors of nano-hole arrays for Label-free bio-detection

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Surface plasmons have received great attention due to their extraordinary optical characteristic. The interaction between metallic thin films consisting of subwavelength nanostructures and lights causes plasmonic resonance. This phenomenon is able to be utilized for many applications such as color filters, image sensors, and plasmonic microscopies [1-2]. Recently, many kinds of nanostructures have been developed for label-free bio-detection [3-5].

In this study, we investigated the contribution of geometric factors to detecting resolutions and found optimized conditions for high sensitivity. To do this, structural color filters (SCFs) composed of 2-dimensional nano-hole arrays were formed on 150 nm-thick aluminum films as following a quadrate arrangement. The hole diameter and spacing varied from 120~220 nm and 260~400 nm with 10 and 20 nm steps respectively. Then, the solutions of collagen and bovine serum albumin (BSA) diluted to 20 $\mu g \cdot ml^{-1}$ with phosphate buffered saline (PBS) were dropped on SCFs to evaluate the role of geometric factors. As a result, improvement of detecting resolution occurred when both hole diameter and spacing increased.

In addition, human embryonic kidney (HEK-293) cells were prepared to confirm the detecting ability of fabricated SCFs and their resolution. Based on the result from simple proteins, in this step, we tried to distinguish nucleus and cytosol from the cell. Owing to their characteristic dielectric constants which are different from each other, it was also expected that the positions of plasmonic resonances are different. This difference makes distinguishable transmission for each unit pixel of optical microscope images. Therefore, instead of complex spectra analysis, color coordinates such as '*Hue*' and '*Lab*' spaces were used. Both parameters presented coordinates which distinguish nucleus and cytosol areas.

According to the result, geometrically optimized SCFs and analyzing method based on color coordinates show possibility that they are suitable candidates for label-free and real-time in-vitro bio-detection.

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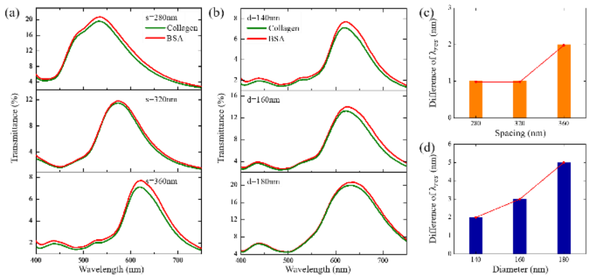

Figure 1. Measured transmission spectra of SCFs with increasing (a) spacing and (b) diameter after proteins were dropped. The difference of the resonance wavelengths are plotted on (c) and (d).

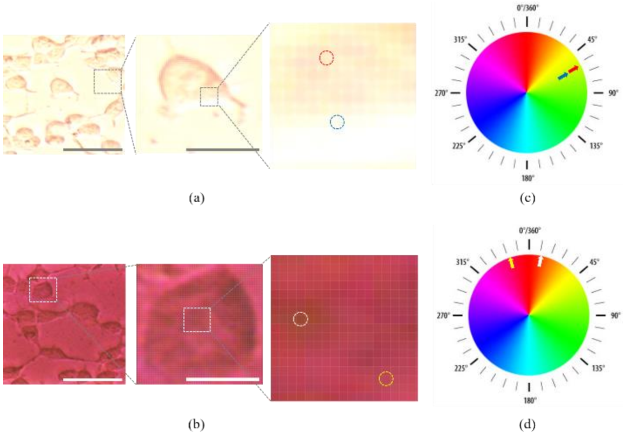

Figure 2. (a-b) OM images of the glass substrate and SCF with HEK-293 cells. (c-d) '*Hue*' color spaces of nucleus and cytosol areas.

Multiplexed sensing of steroids with silicon nanowire field effect transistors

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The simultaneous detection of multiple targets within a single chip on a point-of-care device is a milestone drawing great attention within bio- and nanotechnology areas for more than a decade [1]. Here, we demonstrate a multiplexed, label-free and real-time detection platform for small molecules like hormones and steroids, based on top-down fabricated silicon nanowire-based field effect transistors (SiNW FETs). The honeycomb-structured devices offer noise reduced, versatile and reliable electrical characteristics with high on/off ratios up to 1.7x 10^6 as depicted in figure 1.

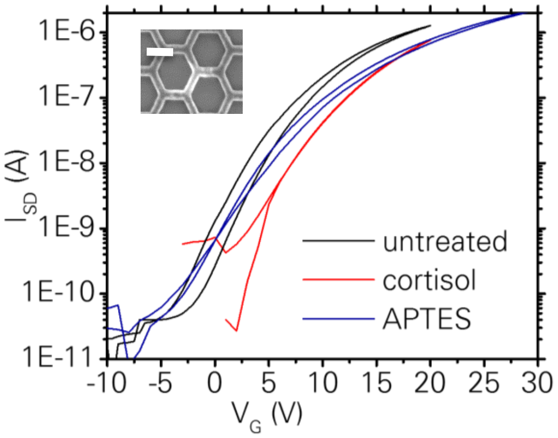

Figure 1. Transfer characteristics of silicon nanowire based field effect transistor upon different surface functionalization. Inset: SEM image of silicon nanowires with a scale bar of 200nm.

Monitoring of steroids plays an important role in the treatment of chronically stressed persons and professional groups, detection of dopants and inherent drug abuse, or simply for hormone screenings. Multiple SiNW FETs connected to a CMOS multiplexor chip enables the readout of up to 32 FETs simultaneously. We particularly focus on the sensitive and selective binding of the targets onto the SiNW FETs by using aptamers as receptors in order to allow high sensitive screenings in more physiological conditions [2]. In order to detect specific targets single FETs are functionalized individually by nanoprinting. Fluorescent microscopy confirmed target- receptor binding directly on the FETs. Figure 2 shows optical and electrical signals taken on the same FET after biorecognition process.

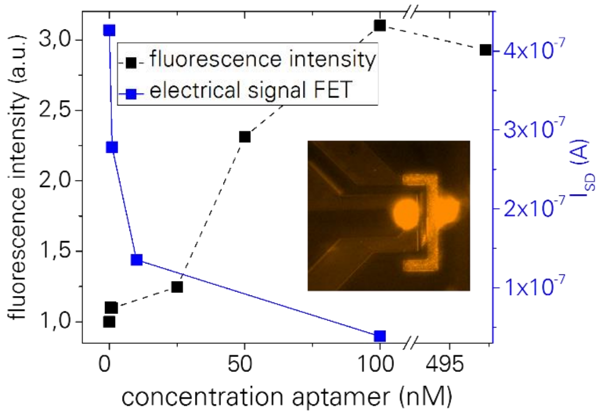

Figure 2. Fluorescence intensity signal of differently concentrated target aptamer on SiNW FETs and corresponding change of source-drain-current of the same FET.

Finally, we show the working multiplexing principle in form of the biochipbox that serves as a portable, electro-microfluidic device allowing the versatile and reliable point-of-care detection of multiple samples on one single sensor device.

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The mystery of semiconductor to metal phase transition in MoS_2 under electron beam

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Recently a phase transition from the hexagonal 1H to trigonal distorted 1T'-phase in two-dimensional (2D) MoS_2 has been induced by electron irradiation [1]. Using density functional theory calculations, we study the energetics of these stable and metastable phases when electric charge, mechanical strain and vacancies are present. Based on the results of our calculations, we propose an explanation for this phenomenon which is likely promoted by charge redistribution in the monolayer combined with vacancy formation due to electron beam and associated mechanical strain in the sample.

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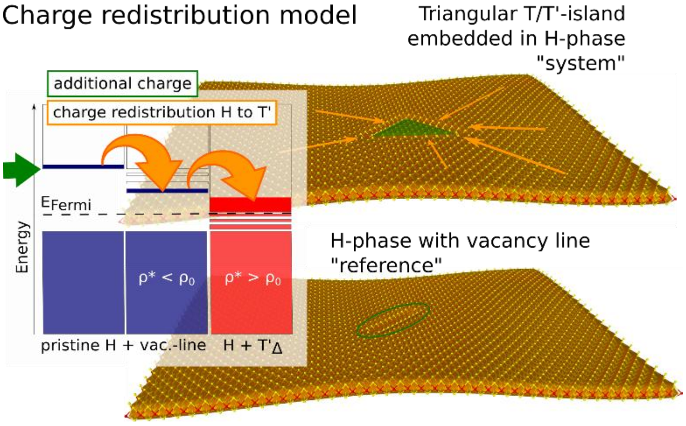

Figure 1. Additional charge initially located in the conduction band minimum is redistributed to the triangular metallic region. This causes the configuration with the metallic region to become energetically favorable over the semiconducting reference configuration with vacancy line.

Doped Single-Walled Carbon Nanotubes for Flexible Thermoelectric Applications

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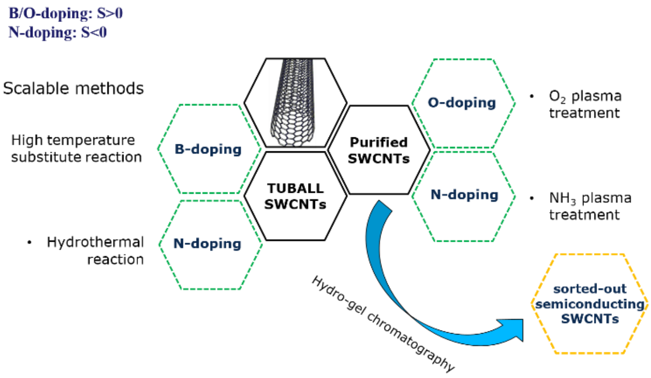
Single walled carbon nanotubes (SWCNTs) have a high potential as flexible thermoelectric (TE) materials owing to their high charge carrier mobility, light weight and outstanding mechanical properties [1]. Recently, purified semiconducting SWCNT films showed TE properties comparable to commercial Bi_2Te_3 alloys [2]. Doping is a crucial step towards TE application of SWCNTs, not only for maximizing their thermoelectric power factor (S2σ), but also for providing n-type nanotubes that are demanded for TE devices (pristine SWCNTs are p-type materials due to oxygen/water absorption). Here doping as well as ambient effects on the TE properties of SWCNTs are investigated. We performed post-synthesis large-scale boron (B-) and nitrogen (N-) doping for commercial unsorted SWCNTs, by high temperature substitutional reaction and hydrothermal reaction, respectively. The maximum achieved dopants concentration were 0.5 at.% for substituting B atoms and 0.4 at.% for quaternary N atoms for B-SWCNT and N-SWCNT samples, respectively. By boron doping, we were able to enlarge both electrical conductivity (up to 250000 S/m) and Seebeck coefficient (up to 30 µV/K) of pristine SWCNTs that ended up at the increase of the power factor to ca. 120 µW/mK^2. On the other hand, a high amount of oxygen absorbed on N-doped SWCNTs is found to be the main obstacle for achieving negative Seebeck coefficient in ambient conditions.

As an alternative route towards improving TE properties of carbon nanotubes, semiconducting (sc-) SWCNTs were sorted out by gel chromatography, and thin sc-SWCNT films were prepared. By separating semiconducting-only nanotubes, Seebeck coefficient of SWCNT samples has been dramatically increased up to 120 µV/K. Then, the sc-SWCNT films were doped by oxygen or ammonia plasma treatment. The treatment with oxygen plasma caused further increase of Seebeck coefficient up to 160µV/K. Ammonia plasma treatment led to a noticeably higher nitrogen-to-oxygen ratio in sc-SWCNTs than in case of the hydrothermal treatment. The films of N-doped sc-SWCNTs are n-type semiconductors with extremely low negative Seebeck coefficient.



Thus, doping of SWCNTs, especially in combination with sorting-out of sc-SWCNTs, leads to a dramatic enhancement of TE properties of carbon nanotubes. It can be expected, that hybrid composites made of doped SWCNTs and polymers may provide a new avenues for the development of optimal materials for flexible TE applications.

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The Study of Physical Properties of Self-Assembled Graphene

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Currently, intensive research taking place in the world to develop simple low-temperature methods for the synthesis of graphene and related materials. This paper considers a synthesis of graphene using colloidal solution of graphite powder (dissolved in water). Also, ultrasonic vibrations were used in the process of synthesis. Obtained layers were substituted on the silicon, amorphous sapphire, monocrystal salt and plastic surface. Scanning electron and atomic force microscopes are used to study surface profile (Fig. 1) and surface potential (by Kelvin-probe method) of samples. The results of surface potential measurements (-400 ÷ -600 mV) are typical for graphene [1]. We also study the change in the surface potential at the graphene-quartz boundary.

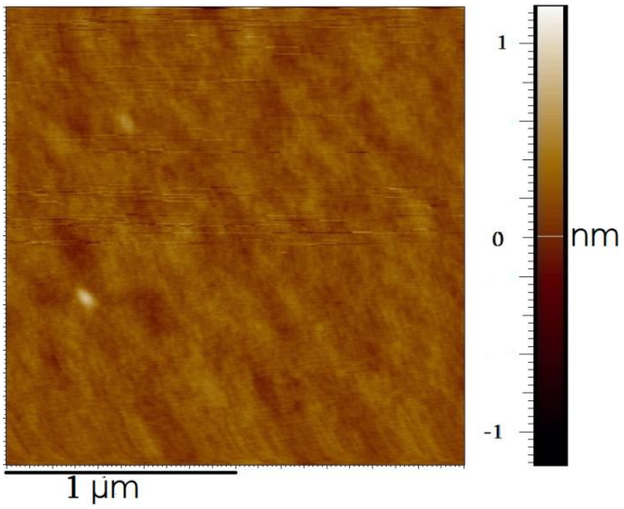

Figure1. AFM image of surface profile of the self-assembled graphene.

In order to elucidate the internal structure of formed films, the Raman scattering and optical absorption spectrums are studied. The joint analysis of the results and reviews the literature [2, 3] indicates the presence of graphene and graphene oxide. When change the substrate (from salt to amorphous sapphire) characteristic absorption peak for graphene shifts to higher energy range, due to the dielectric confinement effect. It happens, because in our case, in addition to the quantum confinement, there is also the so-called dielectric confinement, which is due to the fact that the lines of elektric field between the Coulomb pair (exciton) penetrate to the barier zone and are redistribute. The influence of the effect of dielectric confinement on exitonic absorption mechanism in graphene is discussed too. Also, the current-voltage characteristics of these films are obtained for different values of resistance (Fig. 2). The results are discussed in comparison with the results already published articles [4, 5].

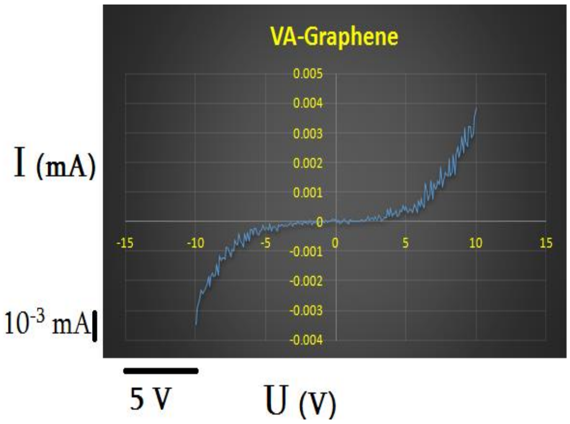

Figure 2: Current-voltage characteristic (for R≈700 kΩ).

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Phononics in two-dimensional materials

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Over the last years, two-dimensional (2D) materials have attracted considerable interest due to the fact that they offer a new broad playground to explore and develop nanoscale devices with tailored electrical, optical and thermal properties [1]. Recently, many prototypes have been proposed for thermal devices (diodes, transistors, and logic gates) based on graphene [2]. Most of these investigations have focused on how to control the heat flux in order to display heat rectification. Moreover, from the point of view of simulating heat transport, it has been shown a great improvement in the development of advanced computational methodologies in order to gain a deep insight into the mechanisms governing thermal transport properties in nanomaterials[3, 4].

Hence, in the present work, we use non-equilibrium molecular dynamics (NEMD) simulations to study the thermal rectification effect in asymmetric MoS_2 and hBN-C nanoribbons. We show that thermal rectification ratios of up to 25 % can be achieved in dependence of the asymmetry degree of the ribbons. It has also been proved that this effect can be tuned by surface engineering. Also, we combine non-equilibrium Green's functions (NEGF) technique with a density functional tight-binding (DFTB) approach to study the influence of diverse factors on the thermal transport properties of novel 2D materials. In the ballistic phonon transport regime, we have found out that the effect of ad-atoms and molecular functionalization on the thermal properties of graphene grain boundaries (GBs) sensitively depends on their structural configuration. Anisotropic thermoelectric properties have been also found in two-dimensional puckered structures. Thermal transport properties have also been tuned by strain engineering in hBN, phosphorene, MoS_2 monolayers, and their corresponding 4|8 and 5|7 grain boundaries.

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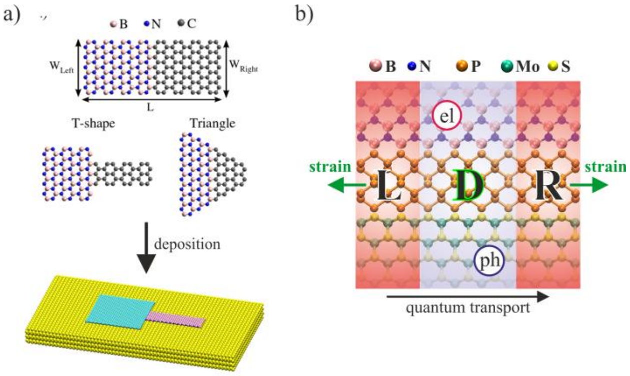

Figure 1. a) Scheme of the deposition on a substrate of thermal diode prototypes made of hBN-C nanoribbons. b) Transport setup for computing thermal transport properties by using NEGF technique.

Direct low temperature growth of vertically oriented graphene nanowalls on multiple substrates by Low Temperature Plasma - Enhanced Chemical Vapor Deposition

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Vertical graphene (VG) is intrinsically graphene, but it also possesses unique structural features, being arranged perpendicularly to the substrate surface. Individual VG nanostructure usually has lateral and vertical dimensions of 0.1 to tens of micrometers and a thickness of only few nanometers. Vertical graphene has a low operating temperature, which can be feasible for industrial applications. Plasma enhanced chemical vapor deposition (PECVD) is a key method for 3D graphene synthesis. The particular PECVD process presented here makes possible graphene deposition without the presence of catalyst and post-transfer treatment. In this study we have used one of the configurations of radio frequency (RF) PECVD: Inductively Coupled Plasma (ICP). As substrates materials we have used conductors and semiconductors. For each substrates we have obtained graphene nanowalls with different structures. The morphological and electrical properties of the obtained graphene nanowalls have been tailored by controlling the growth parameters, such as, plasma power, gas flow, temperature, pressure or cooling time. The characteristics of the VG samples have been analyzed by electrochemical measurements and BET. Also, the quality and porosity of graphene nanowalls have been determined by Raman spectroscopy and Scanning Electron Microscopy.

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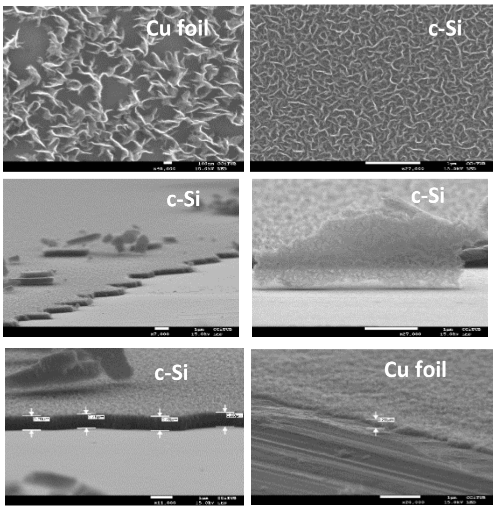

Figure 1. SEM images of VG grown on Cu foil and on c-Si.

Discovery of 2D Mott insulating phase in 1*T*-NbSe$_2$ atomic layer

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Layered transition-metal dichalcogenides (TMDs) have been a target of intensive studies for more than half century since they exhibit a variety of physical properties depending on the combination of elements or the crystal structure such as 1*T* and 2*H* phases [1]. Recent efforts to fabricate atomic-layer counterpart of TMDs gave rise to exotic physical properties distinct from bulk. Among the TMDs, 2*H*-NbSe$_2$ has attracted much attention since it simultaneously exhibits charge density wave (CDW) and superconductivity [2]. In contrast, 1*T*-NbSe$_2$ has not been studied yet because of the difficulty in synthesizing the unstable 1*T* phase [3,4].

Here we report an angle-resolved photoemission spectroscopy (ARPES) study of monolayer NbSe$_2$ epitaxially grown on bilayer graphene. We have succeeded for the first time in selectively fabricating monolayer 2*H*- and 1*T*-NbSe$_2$, and clarified the electronic structure by ARPES [5]. Figure 1 shows the valence-band ARPES intensity plots along the Γ-M cut for monolayer (a) 2*H*- and (b) 1*T*-NbSe$_2$. We found that monolayer 2*H*-NbSe$_2$ exhibits metallic behavior, while 1*T*-NbSe$_2$ shows insulating behavior in sharp contrast to the band theory which predicts the metallic state with half-filled bands. In order to clarify the origin of such unconventional electronic states, we have performed scanning tunneling microscopy (STM). Figure 2 displays constant current STM images of monolayer (a) 1*T*- and (b) 2*H*-NbSe$_2$. We have found that monolayer 1*T*-NbSe$_2$ exhibits CDW with $\sqrt{13} \times \sqrt{13}$ periodicity, distinct from 3x3 CDW in 2*H* counterpart.

In the presentation, we will show detailed ARPES and STM results, and discuss the origin of novel insulating state in 1*T*-NbSe$_2$ in terms of 2D Mott insulating state.

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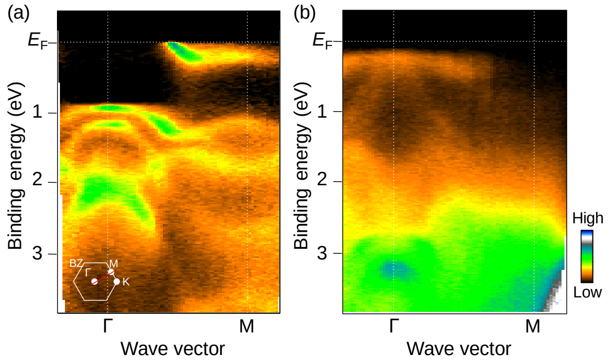

Figure 1. ARPES-intensity plots along the Γ-M direction as a function of wave vector and binding energy for monolayer (a) 2*H*- and (b) 1*T*-NbSe$_2$ at 40 K.

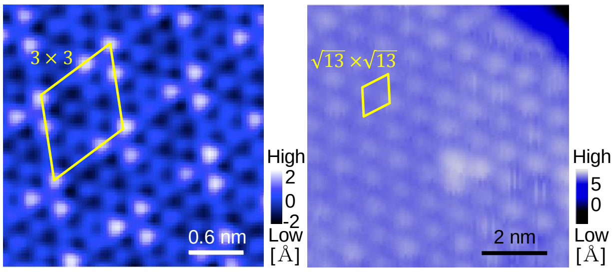

Figure 2. Constant current STM images of monolayer (a) 2*H*- and (b) 1*T*-NbSe$_2$ at 4 K.

Polymer Nanocomposites with Cellulose Nanocrystals made by Coprecipitation

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The reinforcement of industrially produced polymers by way of incorporating micro- or nano-sized fillers is of great interest in material science. Cellulose nanocrystals (CNCs) are rigid, strong, and toxicologically benign nanofibers and have attracted significant interest in this context, due to their facile extraction from renewable bio-sources [1,2]. The commercial production of CNCs has recently been started and CNCs have great potential in applications such as paper manufacturing, composite reinforcement, or rheology modifier. However, one main challenge of using CNCs as reinforcing filler in polymer nanocomposites is to achieve a high level of dispersion in the polymer matrix using established processing techniques [3]. For many industrially produced polymers the direct melt-mixing with CNCs is not satisfying, as it results in composites with large-scale CNC aggregates and limited mechanical properties. For some of these polymers, a homogeneous dispersion of CNCs in the polymer matrix can be achieved by solution casting from organic solvents, but important commodity polymers (e.g. polyolefins such as polyethylene and polypropylene) cannot be solution-cast with CNCs due to their large polarity difference. We report here on two different approaches towards scalable processing of polymer/CNC nanocomposites. In a first approach, we functionalized CNCs with a 2-ureido-4[1H]pyrimidinone (UPy) motif that can serve as a "universal" compatibilizer for CNCs [4]. The motif allows the dispersion of CNCs in both polar (DMF, DMSO) and non-polar (toluene, THF) solvent and thus permits their homogenous dispersion in a great variety of polymers such as polyethylene or natural rubber via solution casting. As an alternative to solution casting, which features disadvantages associated with the drying process, we explored a co-precipitation method, in which polymer/CNC mixtures in a good common solvent were precipitated into water. This process was designed to kinetically trap well-dispersed polymer/CNC mixtures and serves to remove the organic solvent. Indeed, polymer/CNC mixtures thus precipitated form solid beads (Figure 1a), which could be dried and melt-processed using conventional techniques such as injection molding (Figure 1b). Using this process, we prepared nanocomposites of polyurethane with up to 30% of CNCs. A comparison of the mechanical properties of these materials, established by dynamic mechanical analysis and tensile testing, with those of reference materials made by solution casting, revealed virtually identical characteristics.

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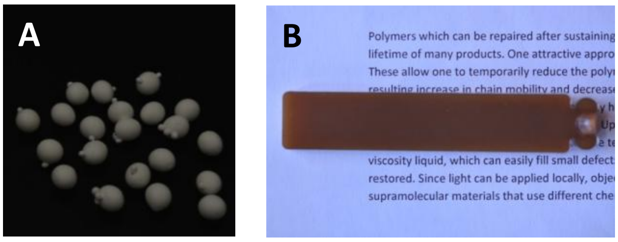

Figure 1. (A) Optical image of polyurethane/CNC beads (10% w/w CNCs) after precipitation from DMSO into water. (B) Photograph of a bar of this nanocomposite made by injection-molding.

Geometrically Enhanced Asymmetric I-V Characteristics in Graphene Tunneling Diode

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Graphene has attracted great attention due to its outstanding intrinsic physical properties [1]. Especially, its high carrier mobility and current density make the graphene as a good candidate for advancing electronic devices such as field effect transistor (FET), diode, RF transmission line, transparent electrode [2-4].

Of them, there have been considerable studies on diode based on the graphene. Although the graphene p-n junction diode has been successfully demonstrated with various doping methods, the rectification properties cannot be observed due to the Klein tunneling phenomena in the graphene. More recently, the graphene tunneling diodes have also been developed based on the van der Walls (vaW) heterostructure method. However, in the tunneling diode, it is hard to get asymmetric I-V characteristics because current flows are originated from the bi-directional tunneling phenomena. Herein, we demonstrated the asymmetric geometries in the graphene for enhancing the asymmetric I-V characteristics in graphene tunneling diode.

Figure1 presents schematics of working mechanism of the graphene tunneling diode and its optical and AFM topography image. The tunneling diode was fabricated with asymmetric geometry to enhance the asymmetrical electrical properties.

2-terminal I-V property of graphene tunneling diode is shown in the Figure 2. At negative bias, the maximum current level is 7.3nA at 3V bias. Otherwise, that of the positive bias is 3.0nA. This asymmetric I-V characteristic is originated from the asymmetrical geometry effects of the graphene.

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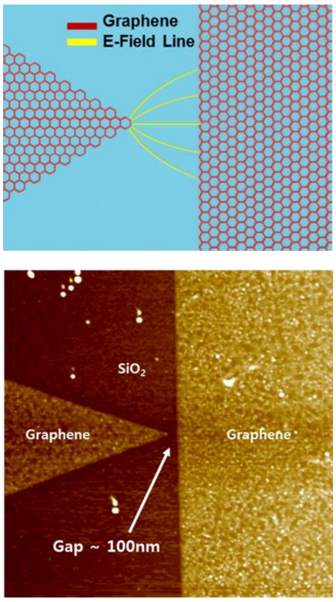

Figure 1. Schematics of the graphene tunneling diode and its working mechanism. The AFM topography image indicates that the fabricated device has 100nm gap.

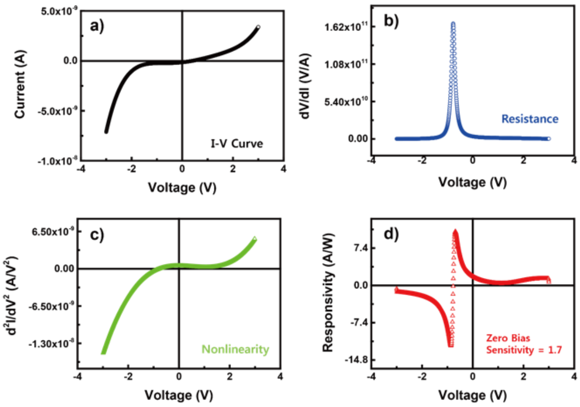

Figure 2. 2-terminal I-V characterisitic of the graphene tunneling diode. The graph shows asymmetric I-V characterisitcs induced by asymmetric geometry effect.

Electrochemical Exfoliation of Layered Conductive Materials

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Graphene and other two-dimensional (2D) materials have led to widespread enthusiasm both in academia and industry. Despite the advantages of these exciting materials have been illustrated everywhere, they have not yet found their way into everyday life products. The major hurdles stand in the reproducible bulk production of high-quality 2D flakes at low cost. Recent discovery reveals that when the layered counterparts are used as working electrode in an electrochemical cell, an electric current drives the migration of ions or charged molecules into the interlayers and pushes thin layers apart. Relying on the rational design of electrolytes and strategies, electrochemical exfoliation can be particularly facile yet efficient with many other advantages such as upscalability, solution processability and eco-friendliness. This talk will focus on our recent progress on the top-down exfoliation of graphite into high-quality, solution-processable graphene flakes on a large scale. Some examples for the application of our exfoliated materials will also be presented.

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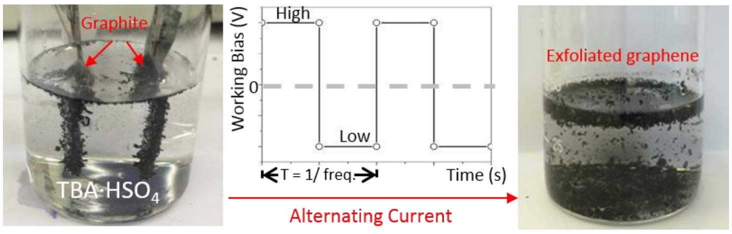

Figure 1. Ultrafast delamination of graphite into high-quality graphene using alternating currents

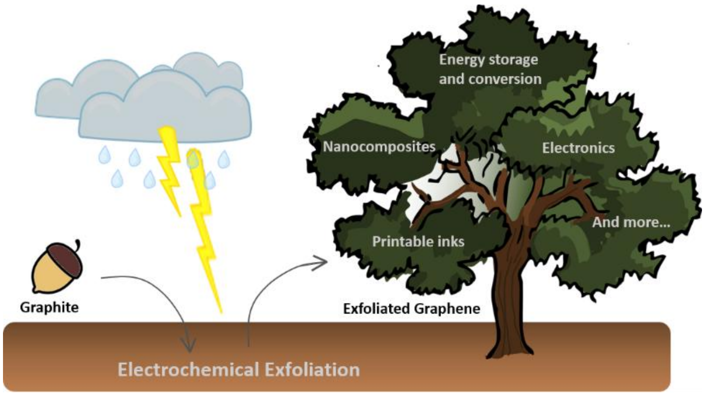

Figure 2. Exfoliation of graphite for a wide spectrum of applications

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One-Pot Reverse Transcriptional Loop-Mediated Isothermal Amplification (RT-LAMP) for Detecting MERS-CoV

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Due to the limitation of rapid development of specific antiviral drug or vaccine for novel emerging viruses, an accurate and rapid diagnosis is a key to manage the virus spread [1]. We developed an efficient and rapid method with high specificity for the Middle East Respiratory Syndrome coronavirus (MERS-CoV), based on one-pot reverse transcription loop-mediated isothermal amplification (one-pot RT-LAMP) [2]. A set of six LAMP primers [F3, B3, FIP, BIP, LF (Loop-F), and LB (Loop-B)] were designed using the sequence of nucleocapsid (N) gene with optimized RT-LAMP enzyme conditions: 100 U M-MLV RTase and 4 U Bst polymerase, implying that the reaction was able to detect four infectious viral genome copies of MERS-CoV within a 60 min reaction time period. Significantly, EvaGreen dye has better signal read-out properties in one-pot RT-LAMP reaction and is more compatible with DNA polymerase than SYBR green I. Isothermally amplified specific N genes were further evaluated using field-deployable microchamber devices, leading to the specific identification of as few as 0.4 infectious viral genome copies, with no cross-reaction to the other acute respiratory disease viruses, including influenza type A (H1N1 and H3N2), type B, human coronavirus 229E, and human metapneumovirus. This sensitive, specific and feasible method provides a large-scale technical support in emergencies, and is also applied as a sample-to-detection module in Point of Care Testing devices.

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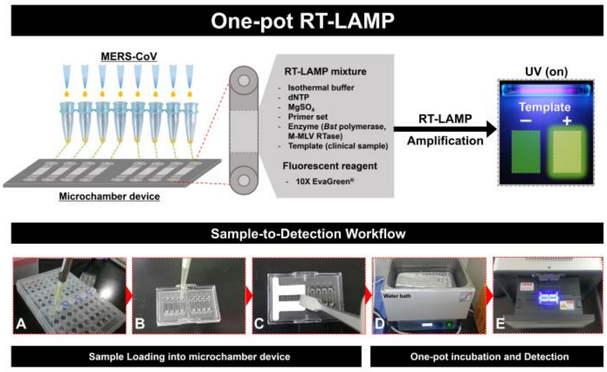

Figure 1. Schematic illustration of the entire one-pot RT-loop-mediated isothermal amplification (RT-LAMP) workflow, "Sample-to-Detection."

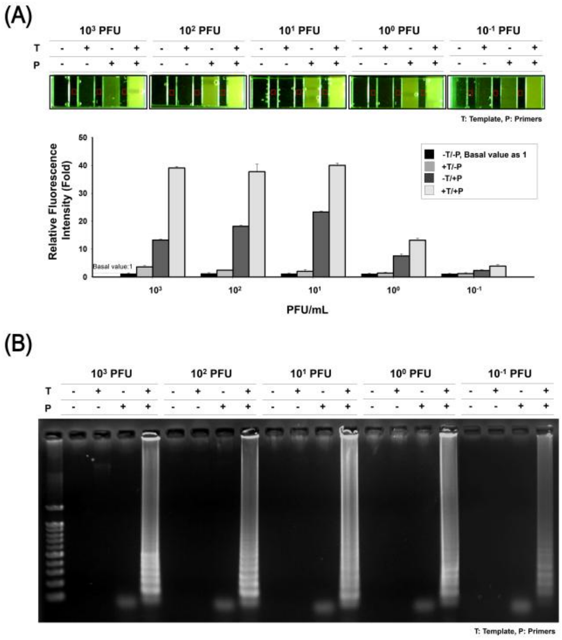

Figure 2. Sensitivity of one-pot RT-LAMP.

Silver Nanoparticles containing Polycaprolactone/Polypropylene Succinate Copolymer preventing microorganism adhesion for wound healing applications

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Wound healing is a pathophysiological process consisting of three overlapping phases of inflammation, proliferation and wound maturation. In these processes, the protection of the wound area from infection is critical for successful maturation and healing. The antimicrobial activity of nanomaterials has been considered an important research area in wound healing process [1]. Antimicrobial nanomaterials are believed to accelerate the healing process by preventing the external inflammation in wound caused by the microbial infection.

In this research, polycaprolactone/Polypropylene succinate/Silver nanoparticle (PCL/PPSu/AgNP) material is proposed for preventing microbial contaminations of a wound area to improve haeling process. First, PEGylated AgNPs were synthesized (Figure 1) and dispersed in PCL/PPSu copolymer structure to gain antimicrobial properties [2]. Antimicrobial activities of the newly prepared structures were then determined by observing the biofilm formation of *S.epidermidis* and *C.albicans* microorganisms and applying plate counting assay [3]. The results of the plate counting and biofilm formation experiments showed that the adhesion of microorganisms to copolymer structure has been substantially prevented by using AgNPs (Figure 2-3). Findings of this study showed the the synthesized copolymer with AgNPs as a promising candidate material for wound healing applications.

Acknowledgements

This study is supported by The Scientific and Technological Research Council of Turkey (TUBITAK) grant number 213M729.

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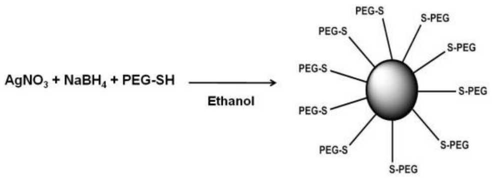

Figure 1. Sythesis of PEGylated silver nanoparticles.

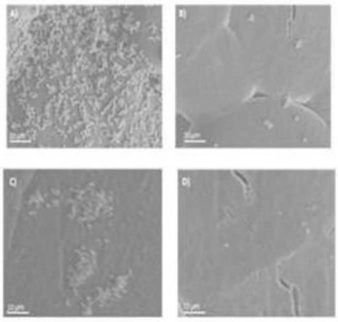

Figure 2. SEM images of the *C.albicans* and *S.epidermidis* adhesion on PCL/PPSu copolymer (A and C) and PEGylated AgNPs containing PCL/PPSu copolymer (B and D).

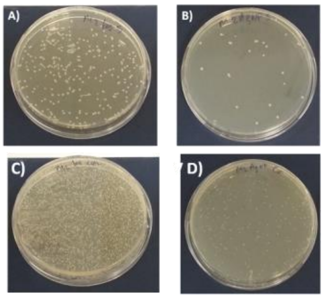

Figure 3. Photographs of the viable colonies which obtained with the plate counting test.

Graphene/Bismuth Selenide Heterostructures for Thermoelectric Applications

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Graphene is modern 2D-material with unique physical properties - optical transparency, high electric and thermal conductivity, mechanical strength and flexibility. Due to these properties graphene is a perspective material for the use as electrode in opto- and thermoelectric devices instead of, for example, widely used indium tin oxide. Hexagonal crystal lattice of graphene is very similar to it of some best thermoelectric materials such as bismuth selenide (Bi_2Se_3). This similarity allows heteroepitaxial growth of Bi_2Se_3 nanoplates on the graphene surface, resulting in formation of graphene/Bi_2Se_3 heterostructures. Previously it was reported that crystallographic growth direction and crystallite size of pure Bi_2Se_3 nanostructures play significant role in improvement of its thermoelectric performance [1]. Likewise, the change of growth orientation of Bi_2Se_3 nanostructures from planar (or epitaxial) to non-planar relative to the substrate surface may enhance thermoelectrical performance of graphene/Bi_2Se_3 heterostructures.

This work is focused on application of vapour-solid deposition method [2] for fabrication of different in terms of continuity and growth orientation types of nanostructured Bi_2Se_3 layers on the surface of monolayer CVD graphene. During Bi_2Se_3 synthesis process short-term inert gas flow was used to change growth orientation of Bi_2Se_3 nanostructures [3]. The relation between synthesis parameters and quality of obtained on graphene surface Bi_2Se_3 nanostructured layers (chemical composition, crystal structure and coverage of graphene area) is discussed. Thermoelectric voltage, generated by obtained graphene/Bi_2Se_3 heterostructures in response to temperature gradient of 16 °C applied to it, is compared. The graphene/Bi_2Se_3 heterostructures, where Bi_2Se_3 layer consisted from both planar and non-planar nanoplates are found to be twice more effective than heterostructures with Bi_2Se_3 layer consisted only from planar nanoplates (Figure 1). Thus, graphene/Bi_2Se_3 heterostructures, where Bi_2Se_3 layer consists of mix of planar and non-planar nanoplates, is perspective material for application in thermoelectric devices.

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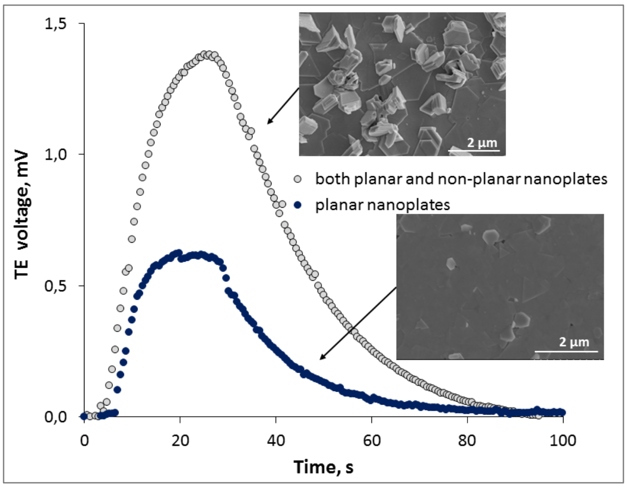

Figure 1. V-t curves illustrating thermoelectric response of the device based on graphene/Bi_2Se_3 heterostructures to the applied temperature gradient of 16 °C for 30 s.

Titanium surface engineering using detonation nanodiamonds towards biomedical applications

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Titanium and titanium-based alloys have been used as implant material for a long time, due to their high ratio of tensile strength and young modulus (σU/E), excellent corrosion properties and high biocompatibility, respectively[1]. The rate and quality of osseointegration in titanium implants are strongly related to their surface properties. In order to improve the biological, chemical, and mechanical properties, surface modification is often performed[2] using various coating materials.

We propose denotation nanodiamonds (DNDs) as a coating material for biomedical applications, due to their nontoxicity, structural and surface properties. According to the high variety of functionalization possibilities DNDs can be integrated in composites, biological systems, electronics, and surface technology[3]. The Fig. 1 shows two innovative approaches: (A) enhanced biocompatibility of metallic implant materials using hierarchical structures of DNDs. These micro- and nanostructures, created by photolithography based processes, will improve the cell attachment. A possible solution to reduce the healing time of implants is shown in approach (B). The first stage contains the establishment of an anodic oxide layer with intrinsic homogenously distributed DNDs. Afterwards, bioconjugated DNDs will be attached to this oxide layer. Promising candidates for a biofunctionalization of DNDs are growth factors, antibiotics and antimicrobial peptides (AMPs). AMPs offer an alternative strategy to conventional antibiotics with a broad-spectrum activity (antibacterial, antiviral and antifungal) and a rapid onset of killing[4].

These hypotheses will be verified experimentally using osteoblast migration, proliferation and differentiation tests. In the first stage structural investigations were conducted. We are going to present the first outcomes regarding properties of the DND coating suspensions as well as DND surface chemistry and DND coating topography. The used methods are zeta potential and dynamic light scattering measurements, infrared spectroscopy as well as SEM top view of DND coatings.

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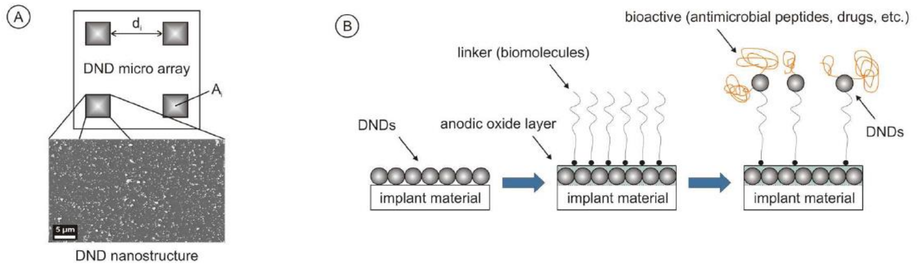

Figure 1. (A) Nano- and microstructuring of Ti using DNDs with various structure sizes Δd_i or array areas ΔA_i, respectively (B) Bioconjugated DNDs covalent attached to an anodic oxide layer with incooperated DNDs[5] to enhance the implant material surface properties.

Nanorotor driven by single-electron tunneling

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Much effort has been devoted to investigate the coupling of electrical and mechanical degrees of freedom on the nano-meter scale in order to design novel electronic devices. An example is the nano-mechanical single-electron transistor (NEMSET), where electrons are transported from a source to a drain electrode via a movable nano-object which can be occupied by exactly one electron. The charged object experiences a force caused by the electric field between source and drain. The interplay of vibrational motion of the particle and the strong distance dependence of tunneling (which is responsible for charging/decharging) gives rise to mechanically assisted electron transport, called electron shuttling.

Recently, we investigated a nano-rotor based on the same mechanism as the electron shuttle described above [1]. This rotor exhibits novel effects, which could be used for various applications, like sensors or charge pumps. The coupling of mechanical motion and tunneling leads to the self-excitation of oscillatory motion and for large bias voltage to rotational motion even in the presence of damping.

A rotor with tilted and unequal arms can rotate preferably in one direction independently on the initial condition [2]. This can be an advantage compared to some previous proposals of nano-motors driven by single electron tunneling because control over the initial condition may be difficult or even impossible, depending on the specific experimental setup. We show which geometries lead to a preferred rotational direction and how stable they are under fabrication imperfections.

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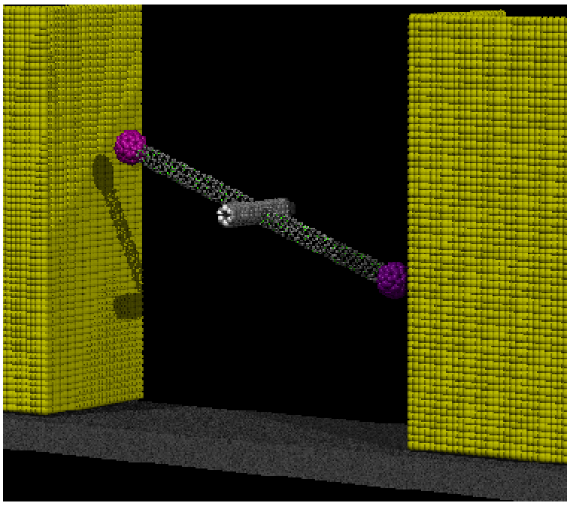

Figure 1. Sketch of a nano-motor realized by a carbon-nanotube.

Performance Of Functional CuO Nanoparticles As Photo-Catalysts For Elimination Of Persistent Dyes In Water

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Metal and metal oxide nanoparticles have deserved considerable attention in the last decade as advanced materials for photocatalytic transformation of pollutant dyes in waters [1]. The presence of persistent dyes in water is of major concern not only because of their colour, but also due to the inherit risks (toxic, mutagenic, carcinogenic) that the dyes present themselves and their breakdown products pose to aquatic life forms.

In this work, we describe the synthesis of CuO nanoparticles (CuONPs) and their surface modification by attachment of hydrocarbon chains using two different long chain precursors (C_8 and C_{18}) with the aim to evaluate their potential as catalysts and photocatalysts for degradation of Congo Red [Figure 1a], a model persistent and mutagenic dye in waters, which is also known to be metabolized to the carcinogenic bezidine [2].

The synthesized raw and functional CuONPs were characterized by FTIR, XRD, TEM, HTREM, and TGV. As can be seen [Figure 1b], HRTEM images of functional $CuOC_{18}NPs$ revealed that their surface was coated with a heterogeneous layer of hydrocarbon chains. On the other hand, TEM images and XRD analysis of CuONPs demonstrated that individual nanoparticles are prolate spheroids with an average length of 20 nm with a 5:2 aspect ratio.

The performance as catalyst of raw CuONPs, $CuOC_8NPs$ and $CuOC_{18}NPs$ was evaluated by UV-Vis spectrophotometry with the aid of UV radiation and its absence, and the kinetics of the processes were measured as well [Figure 2]. The degradation experiments were also performed in absence of NPs and a decrease in the Congo Red concentration was not observed. These results are promising for degradation of Congo Red with less toxic functional CuO nanoparticles.

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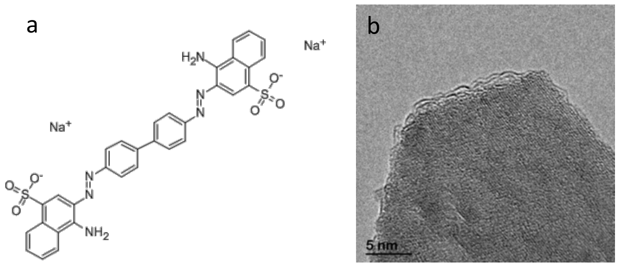

Figure 1. a. Congo Red structure b. HRTEM image of Functional CuO nanoparticle. $CuOC_{18}NPs$.

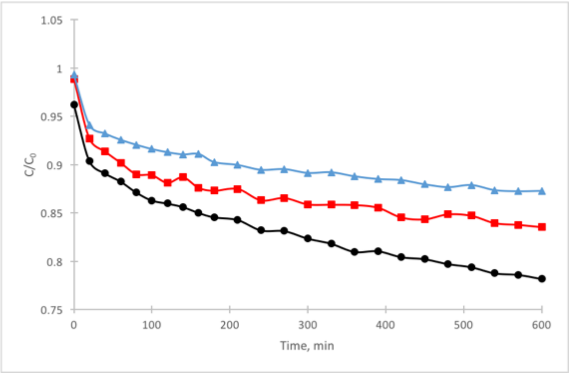

Figure 2. Kinetics of the Congo Red elimination in absence of UV radiation by treatment with (●) CuONPs, (■) $CuOC_8NPs$ and (▲) $CuOC_{18}NPs$.

Development of Functional Electronics Integrated to 3D Structures via Material Extrusion Printing Process

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Functional electronics are fabricated by printing plastic and metal material using material extrusion printing process. User interface unit including external case and assemble guide is fabricated for the exterior of the functional electronics. Electronic circuit to deliver power to the electronic components and battery slot are fabricated for the interior of functional electronics. New functional electronics are printed right after printing process. The plastic material is adopted for the electronic structure, and the electronic circuit is fabricated by printing a conductive material on the electronic structure. Electronic circuit design including wiring between electronic components on a 3-dimensional structure should be preceded, and electrical wiring is formed simultaneously with printing the conductive material. Conductive polymer and eutectic alloy are used for the conductive materials. The characteristics of 00(unknown) were analyzed and applied to the process parameters for the material extrusion printing process. Each conductive materials had a wide specific resistance variation from hundreds mΩ ·㎝ to tens μΩ ·㎝ at same printing parameters. The conductive material is not necessary to post process and is suitable for printing process which immediately fabricates outputs by demonstrating the electrical performance of the electric circuit. Circuit fabrication technology that is not constrained to the boundaries of the dimension is expected to increase the use of 3D printing technology in the electronics industry.

Figures

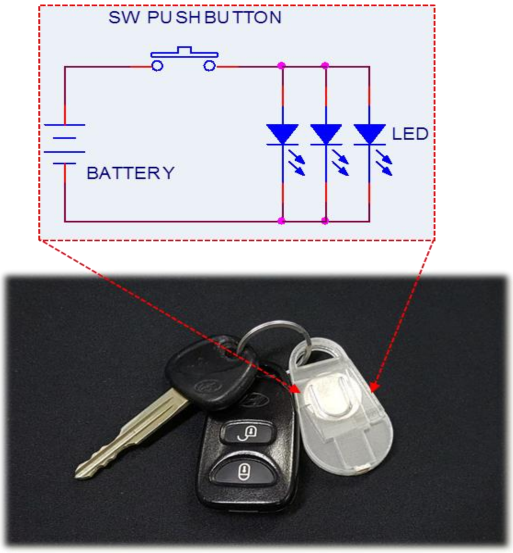

Figure 1. Fabricated of LED circuit integrated plastic keychain.

Monte Carlo simulations of 2D molecular self-assembly

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Controlling the formation mechanism of organic thin films (OTFs) tailored by weak interactions on van der Waals (vdW) substrates provides an opportunity to obtain highly stable, large-area, and high-quality organic electronic devices [1]. To this end, understanding the self-assembly of organic molecules, like pentacene, from a disordered state into ordered 2D crystals is of great importance.

We use classical Monte Carlo simulations in order to study the growth of OTFs on monolayer substrates (graphene, hexagonal boron nitride). We investigate the intrinsic driving mechanisms responsible for the molecular ordering and analyze the role of the substrate for the growth process. In particular, we are address the question of controlling the orientation of the molecules. Further, we study the influence of temperature on the resulting aggregates. Our work complements a recent study based on molecular dynamics simulations [2].

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Figure

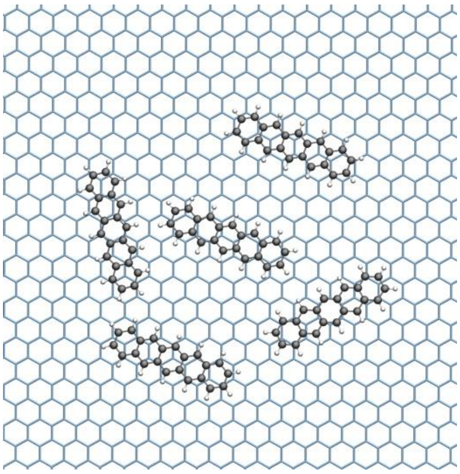

Figure 1. Intermediate step of the self-assembly process of pentacene molecules on a graphene substrate (schematic).

Seedless Synthesis of Gold Nanorods: Some Features and Benefits

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Gold nanorods (GNRs) are of considerable interest for solving of various nanoplasmonics' problems [1]. This is due to the possibility of fine tuning of GNRs longitudinal plasmonic band in the near IR region by varying their aspect ratio. Conventional approach to the GNRs creation implies the preliminary synthesis of Au seed nanoparticles and their subsequent growth in "soft templates" – cetyltrimethylammonium bromide (CTAB) micelles [2]. Its main drawback is high sensitivity to the quality of the reagents (especially CTAB) [3]. Moreover, the GNRs yield crucially depends on medium pH, temporal stability of seeds and other experimental conditions.

Recently a significant interest is caused by the alternative route – so-called seedless synthesis. In this case, the seed nanoparticles are generated directly in the reaction mixture [4].

The goal of this study is careful examination of the peculiarities of GNRs seedless synthesis in CTAB micelles using the hydroquinone as reductant.

The influence all of the reactants on the yield and plasmonic properties of GNRs is analyzed.

A nonmonotonic dependence of position of GNRs longitudinal plasmonic band on hydroquinone concentration is revealed. The hydroquinone impact on the structure of micellar template is discussed.

The possibility of fine tuning of GNRs longitudinal plasmonic band by temperature variations is demonstrated for the first time. The preliminary data on evolution of plasmonic characteristics of GNRs during their growth are obtained.

This work was supported by the Presidium of Russian Academy of Sciences within the program Basic Research no. 1.8P.

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Imaging and manipulating different supramolecular assemblies of acetylbiphenyl with a four-probe scanning tunneling microscope

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The controlled manipulation of nanostructures is of importance for the construction of molecular devices. Here, we use a low temperature ultrahigh vacuum four-probe scanning tunneling microscope to study acetylbiphenyl (ABP) molecules on Au(111). ABP forms different supramolecular assemblies via hydrogen bonds on the surface. The tetrameric structure and a trimeric structure can be controllably moved several nanometers by voltage pulses. [1, 2] In this work, we discuss the dependency of the movement on the polarity and location of the applied voltage pulse on the different assemblies. Scanning and manipulating with all other tips at the same time is possible without influencing this manipulation.

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Figures

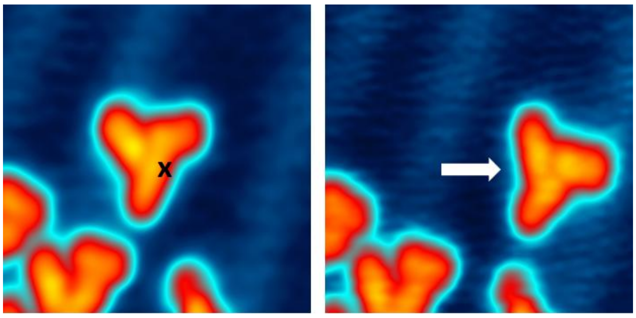

Figure 1. An ABP-trimer controllably moved on Au(111) by using a voltage pulse. The assembly laterally moved and rotated after the pulse.

Docetaxel-loaded PEGylated liposomes development using factorial design

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Docetaxel (DTX) is an anticancer drug, but low solubility and bioavailability limit its application. Within this context, liposomes, nanometric lipid vesicular systems, enable encapsulation of drugs, with several advantages, including protection against degradation, sustained drug release and improvement of pharmacokinetics [1]. However, docetaxel-loaded liposomes based on soy phosphatidylcholine (SPC), cholesterol (Chol) and 1,2-distearoyl-sn-glycero-3-phosphoethanolamine-N-[amino(polyethylene glycol)-2000 (DSPE-PEG(2000)) prepared under high pressure homogeneization have not been reported. Noteworthy, development of formulations by factorial design enable reduction of experiments and determination of optimum variables. For formulation preparation, the hydration of the thin lipid film was employed. Briefly, lipids and drug were solubilized in chloroform in a round-bottom flask and solvent was evaporated under rotary evaporation. Then, the lipid film was hydrated with pH 7.4 PBS buffer at 60°C, followed by homogeneization under high pressure (10000 psi for 20 min). Lipid to drug ratio (10:1, 20:1 and 30:1), Chol:lipid ratio (1:10, 2:10 and 3:10) and DSPE-PEG(2000) mol% (2.5, 5 and 7.5%) were variables studied in order to obtain liposomes with minimal nanometric size and polydispersity (PdI) and maximum encapsulation efficiency, using a Box-Behnken Factorial Design (Minitab Software). Particle size, PdI and zeta potential were evaluated through Dynamic Light Scattering (DLS). Encapsulation efficiency (EE) was assessed using a validated analytical method, based on High Efficiency Liquid Chromatography (HPLC), employing a 250 mm C-18 chromatographic column, mobile phase composed of water:acetonitrile:methanol (35:15:65) at a flow rate of 0.8 ml/min and detection using wavelength at 232 nm. Results showed that particle size, PdI and zeta potential were not statistically dependent on the tested variables. Liposomes had particle size varying from 59.85 ± 0.51 to 144.67 ± 39.49 nm, values suitable for parenteral administration, and PdI ranging from 0.18 ± 0.005 to 0.55 ± 0.013. Zeta potential ranged from -10.7 ± -0.47 to -26.9 ± -0.72 mV, which is acceptable for colloidal stability. Additionally, encapsulation of DTX was adequate, with efficiency varying from 68.56 ± 10.98 to 99.45 ± 2.36%. It was observed a statistically relevant relationship between EE and lipid:drug ratio ($p < 0.05$, using the square method of analysis of variance) and, overall, higher ratios were correlated with better values of encapsulation, as expected (Figure 01). Using the response optimizer tool in the software, the best formulation for maximum encapsulation efficiency should be prepared using lipid:drug ratio at 22.93, Chol:lipid ratio at 0.2 and DSPE mol % at 7.5. In conclusion, only the lipid:drug variable affected DTX encapsulation. Furthermore, the formulation developed herein using factorial design is promising for further physicochemical characterization and evaluation regarding its anticancer properties.

Figure

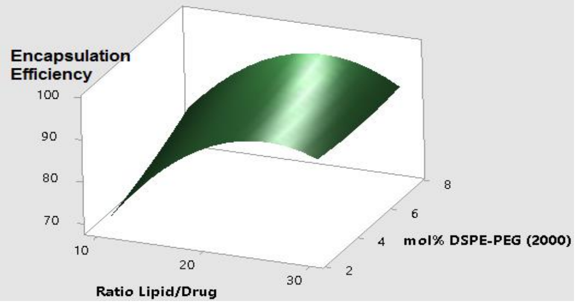

Figure 1. Surface plot of encapsulation efficiency vs lipid/drug ratio and mol% DSPE-PEG(2000)

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Carbon dots as additives in lubricant oils

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In mechanical systems, consistent performance and energy saving demand eco-friendly and highly efficient lubricants. In today's market, 90% of lubricants are composed of hydrocarbon molecules and the rest are additives governing their behavior. In the last decade, it has increased the development of organic-inorganic hybrid lubricants by introducing nanoparticles within the base oil.

Most developments have used inorganic nanoparticles such as ZrO_2, CuO, ZnO, etc [1,2]. These nanoparticles have the disadvantage of forming non-stable suspensions in lubricant oil due to their hydrophilic surface. Often surfactants are added to enhance dispersion or, otherwise, attaching to the nanoparticle surface hydrophobic groups.

Carbon nanomaterials (carbon nanotubes, fullerene, graphene) have attracted much attention due to their unique physical and chemical properties, among which carbon nanotubes have been used as excellent additives in base lubricant oils to improve their tribological performance.

In this presentation we describe the synthesis of carbon-dots (carbon nanoparticles) from citric acid and glutathione by a hydrothermal carbonization method [2] and their surface functionalization with sodium trifluoromethane-sulfonimide (Figure 1). These nanoparticles were characterized in TEM FTIR and solid RMN.

The effect of concentration and morphology of nanoparticles suspended in lubricating oils was examined. Different dispersions were prepared by mixing the raw and the functional carbon dots with mineral oils. The lubrication performance of the dispersions was evaluated using ball-on-plate and three-point contact (ASTM 4172-94 standard test) configurations under various normal forces.

Preliminary tribological results indicated reduced wear compared with the base oil only, while friction coefficient was similar to that of the base oil (Figure 2).

These results reveal that carbon dots may act as suitable materials which could improve lubricant behavior of conventional oils. More work is in progress in order to optimize functionalization of carbon dots, size and concentration, key parameters affecting wear and friction reduction.

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Figures

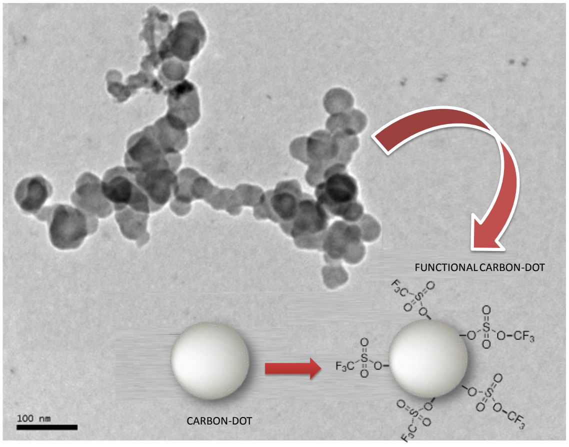

Figure 1. TEM image of functional carbon-dots.

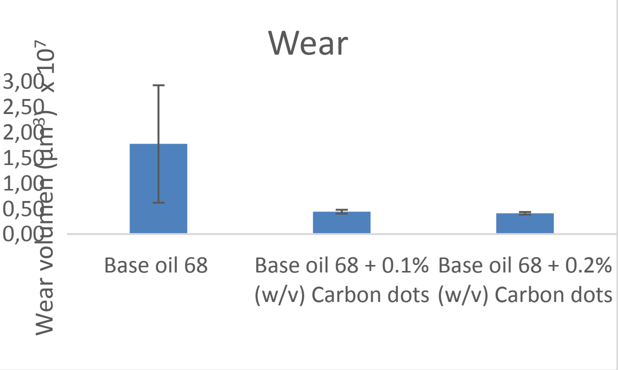

Figure 2. Wear after ASTM 4172-94 standard test of base oil and raw carbon dots.

Label-free detection of DNA sequences derived from avian influenza virus H5N1 using carbon nanotubes

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Victor Romay[1], Bergoi Ibarlucea[1,2], Larysa Baraban[1,2], Vyacheslav Khavrus[1,3], Viktor Bezugly[1,2], Gianaurelio Cuniberti[1,2]

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Avian influenza virus (AIV), especially highly pathogenic AIV H5N1 has become nowadays a very dangerous pathogen threatening not only for poultry but also for human [1]. In this study, we developed and tested chemiresistor type DNA sensors based on semiconducting single walled carbon nanotubes (sc-SWCNTs) as well as on nitrogen doped multi-walled carbon nanotubes (N-MWCNTs) for highly efficient and fast detection of AIV H5N1 DNA sequence. The sensors based on N-MWCNTs were fabricated with direct contact printing of vertically-grown nanotubes where both rigid and flexible target substrates were employed (Fig. 1a) whereas sc-SWCNTs were produced by epitaxial elongation of short fragments of selected sc-SWCNTs on quartz substrates (Fig 1b). Both N-MWCNTs and sc-SWCNTs were functionalized with single stranded DNA probe sequences, which were non-covalently attached to the nanotube sidewalls; the sensing is based on the resistance change after DNA probe detachment when hybridized with complementary DNA sequence (DNA T), see Fig. 1c. The sensors could reliably and quantitatively detect AIV H5N1 DNA in dry conditions and at room temperature. The lowest reliably detected concentration of DNA T sequence was 20 pM for N-MWCNT and 2 pM for sc-SWCNT sensor after 15 min of incubation (Fig. 1d and 1e, respectively). Our CNT based DNA sensors are small, flexible, easy-to-use as well as highly sensitive and selective that makes them promising in clinical diagnostics and for portable applications.

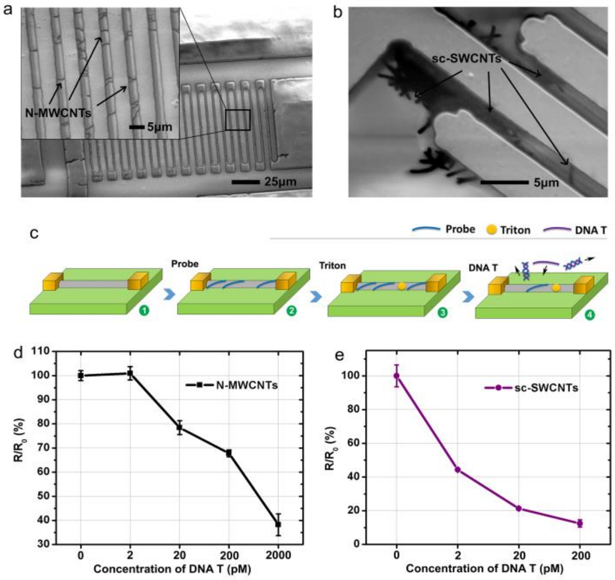

Figure 1. **(a)** SEM image of N-MWCNT based chemiresistor sensor device, the inset shows a regular array of horizontally aligned N-MWCNTs bridging interdigitated electrodes. **(b)** Low-voltage SEM image of patterned interdigitated electrodes bridged with sc-SWCNTs. **(c)** Schematic illustration of the CNT-based chemiresistor DNA sensor functionalization and sensing steps. Resistance change of **(d)** N-MWCNT and **(e)** sc-SWCNT based sensors as the response to increasing concentrations of DNA T (at V=2.0 V) count with respect to resistance value at 0 pM (no DNA T).

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Challenges in the fabrication of devices grown by Molecular Beam Epitaxy

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Scientists around the world demand for high quality and reproducible samples. For the fabrication of tailored devices, molecular beam epitaxy (MBE) has become the method of choice for many universities [1, 2]. In the field of research MBE offers multiple advantages compared to production techniques like chemical vapor deposition, sputtering or liquid phase epitaxy.

One of the main advantages is the flexibility and high adaptability to address the different needs of growth for various devices: microcavities for cavity quantum electronics and light-matter coupling [3], organic and inorganic nanostructures for novel optical devices [4] as well as topological insulators for fundamental research [5].

We like to focus on typical questions and challenges which arise during the growth of high quality samples with molecular beam epitaxy. The questions on the one hand are related to the system and affect the desired homogeneity profile (Figure 1) and wafer temperature uniformity. Challenges on the other hand are influenced by the increasing requirements for high-precision and reproducible samples. In order to reach these requirements we need to push the physical limit set by the MBE-system. Background-doping, shutter transients and defect density are typical concerns which need to be addressed.

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Figures

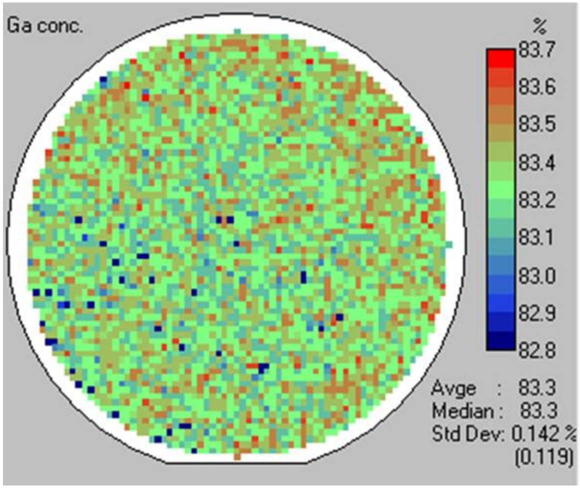

Figure 1. Room Temperature Photoluminescence Map of a thick InGaAs layer on a 3” wafer proving negligible compositional variation of Indium and Gallium across wafer

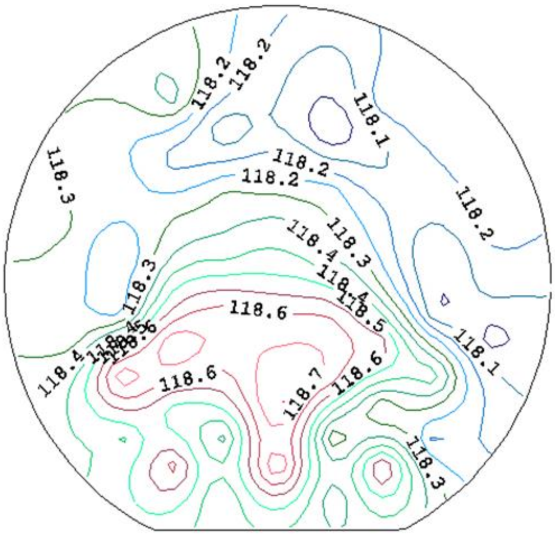

Figure 2. Silicon Doping Uniformity map on a 3” wafer generated from 55 test points. Since Si doping is fairly insensitive to growth conditions, the test is good representation of flux uniformity which shows a standard variation of 0.19%.

Density Functional Tight Binding Method for Plasmonics

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Electrodynamics methods have been proved to be useful and powerful tools to theoretically study localized and delocalized surface plasmons [1]. The recent progress achieved in fabrication techniques to control subnanometer structures and features has lead to search for more rigorous approaches able to theoretically describe nonlocality or the spill-out of conduction electrons, effects well visible in very narrow junctions or subnanometers gaps [2].

Standard atomistic ab-initio *Time-Dependent Density Functional Theory* (TD-DFT) is the most suitable approach for a complete quantum mechanical treatment of plasmons [3] but it becomes computationally unaffordable for particle sizes of several hundreds of atoms.

Here we alternatively propose a *Time-Dependent Density Functional Tight-Binding Method* (TD-DFTB) study [4] on silver dimers done using an optimized Slater-Koster parametrization. More in detail, we study the plasmonic response of dimers of closed-shell Ag$_n$ (n=10, 20, 35, 56, 84 and 120) tetrahedral clusters (tip-to-tip configuration) as well as Ag$_{116}$ cuboctahedral clusters (face to face configuration) as a function of the nanogap size (from 2 Å to 20 Å). Atom positions are fixed to the ones obtained by relaxing the isolated clusters within standard DFT (TURBOMOLE code) and geometries are re-optimized only for the smallest gaps (2 Å and 4 Å).

A red-shift in the plasmonic peak can be clearly seen in Fig. 1 by reducing the interparticle distance until 6 Å, this being due to the clusters mutual depolarization. For smaller distances, a blue-shift effect appears for both the structures, this proving the onset of a quantum mechanical effect already evidenced in literature within other approaches [5]. Moreover, it should be noted as the coupling effects, both in the near-field and in the near-touching regimes, become stronger as the number of interacting atoms becomes larger (Fig. 1b). With a computational cost much smaller with respect to standard TD-DFT one, TD-DFTB seems thus to be a useful method to overcome the limits of classical description and thus to favor the spread of computational quantum plasmonics.

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Figures

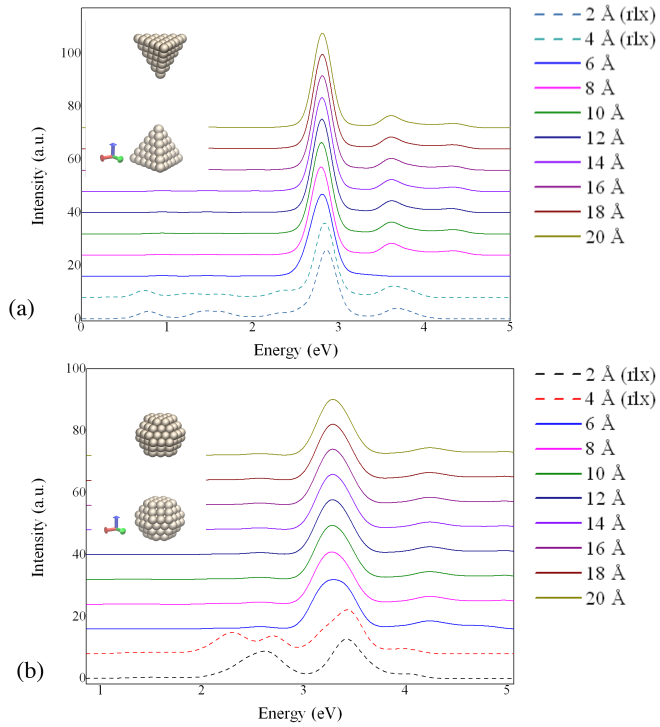

Figure 1. TD-DFTB efficiency calculated for dimers of tip-to-tip closed-shell Ag120 tetrahedrons (a) and face-to-face Ag116 cuboctahedrons (b). Separation gaps from 2 Å to 20 Å are analyzed with the spectra reported from the bottom to top side of the panels, respectively. Geometries are sketched in the insets.

Synthesis, Characterization and Application of WS_2 nanostructures in Gas Sensing

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WS_2, is one of the most promising 2-D materials for gas sensing applications after graphene [1]. In the current study, WS_2 nanostructures were synthesized by a simple and relatively low temperature colloidal route in the presence of oleylamine (OLA). The formation of nanosheets was found to be a function of time from nanoflakes to nanosheets (fig. 1). The diffraction pattern showed prominence of the (002) peak suggesting the existence of multi-layered nanosheets (fig. 2). The nanostructures displayed an n-type behavior towards certain polar and non-polar chemical vapors.

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Figures

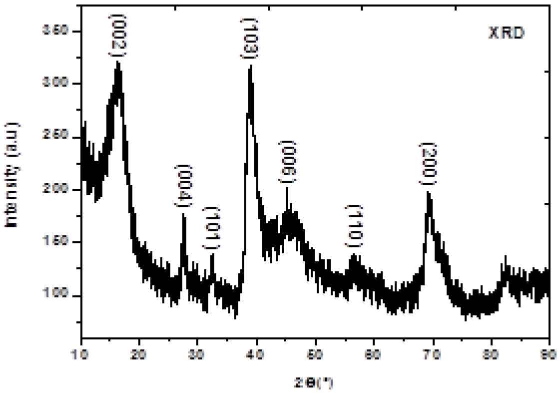

Figure 1. Typical XRD pattern of WS_2 nanosheets

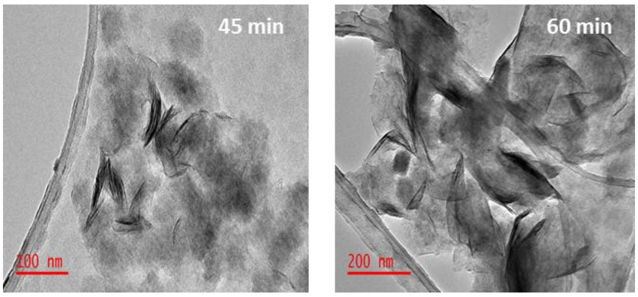

Figure 2. Typical TEM images of WS_2 nanostructures at different reaction time intervals

Influence of channel morphology on CNTFET device performance

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Enhancement of carbon nanotube based field-effect transistor (CNTFETs) performance for high frequency analog electronics goes inevitable along with an increase in the density of semiconducting nanotubes [1, 2]. However, with increasing density device performance is more and more determined by shielding and bundeling issues [3]. In this paper we unfold the influences of channel morphology by a systematic study on two different sets of FET structures correlating morphologic and electrical characteristics as well as changes after thermal annealing. In addition, simulations have been performed to support the experimental findings. It revealed a diversified picture on FET performance under different structural situations.

In Fig. 1, transfer characteristics of CNTFET-d (debundled) and CNTFET-b (bundled) devices including the state before and after annealing are compared. As expected, on-conductance (G_{on}) increased after annealing due to the reduced Schottky barrier and improved current injection. While in the as-prepared state both FET configurations indicate gate control of devices, the transfer characteristics dramatically change after annealing indicating different environmental and structural situation. Since removal of contaminants along with rinsing is expected to be less efficient in bundled CNT assembles, assembly structure should be directly interrelated to interface configurations with respect to doping and proximity effects. In addition, measuring the device under atmosphere lead to a water-induced doping. It can be assumed that spacing in bundled as well as closely packed CNTs is reduced by the annealing which eventually reduces gate control in conjunction with the CNT doping. The strong shift of V_{th} seen for the bundled CNTs in the experiment, can be explained by an effective increase of the impact of doping due to the proximity of CNTs after annealing. This has been confirmed by the simulations as shown in the inset in Fig. 1b. Thus, a higher $+V_{GS}$ is required to deplete all injected charges and completely switch off the device, which results in a shift of the transfer characteristics curves more into the positive gate voltage. In conclusion, this study shows that contaminants and water-induced doping has a much larger impact on the device characteristics especially in the subthreshold region and for V_{th} in case of tube bundles. This emphasizes that especially in dense s-SWNT assembles bundling has to be suppressed to enable removal of all contaminants at interfaces in order to get reproducible and stable device characteristics.

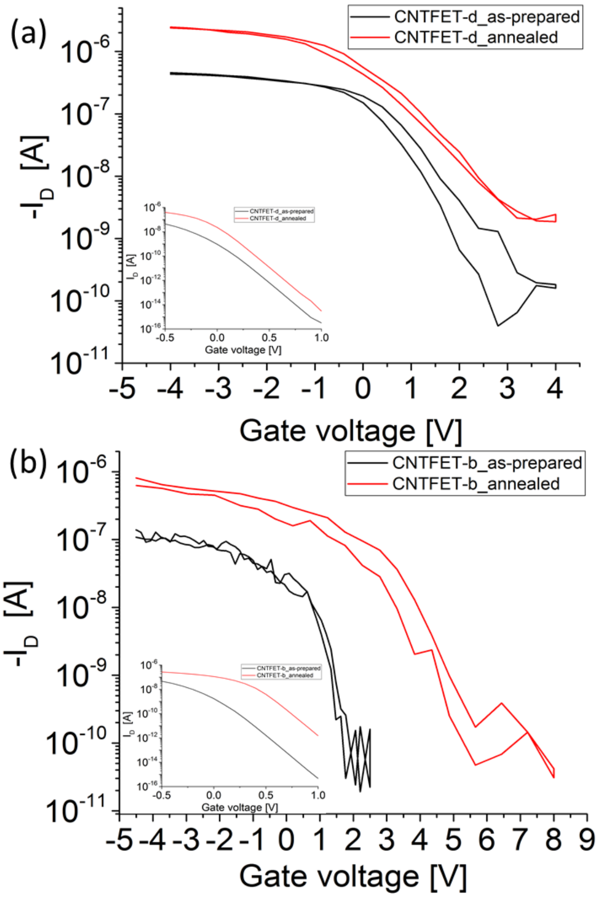

Fig. 1. Transfer characteristics of FETs comparing as-prepared and annealed state of FETs with (a) debundled and (b) bundled nanotubes. Figure inset show the results obtained from the simulation.

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CuO nanoparticle composite structures with carbonnanotubes

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Multiwalled carbon nanotubes (MWCNT) were grown on the Cu foil substrates by electrophoretic deposition (EPD) method. It is shown that the CNT distribution on the Cu substrates greatly depends on the applied voltage and the solvent type such as, deionize water, acetone or triethylamine. XPS measurements have shown formation of CuxOy for the CNT growth in each solvent type. Highly homogeneous CNT deposition on the Cu surface has been achieved by acetone solution within a shorter time. Also, it is observed that the amount of oxide in the structures produced in the acetone/CNT solution is less confirmed by the X-ray Photoelectron Spectroscopy (XPS) analysis.

Annealing at higher temperatures of those Cu/CNT structures gives rise to CuxOy nanoparticles formation together with CNT. Also, by annealing at relatively high temperatures around 900 ^{0}C Cu/CuONP/CNT composites structures are formed. It is seen that CNT structures becomes graphitic like structures covered by CuO NPs under high temperatures annealing.

Figures

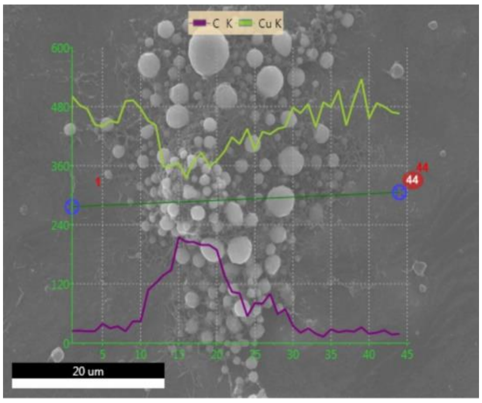

Figure 1. SEM images and EDAX line analysis of Cu/CuONP/MWCNT composite film

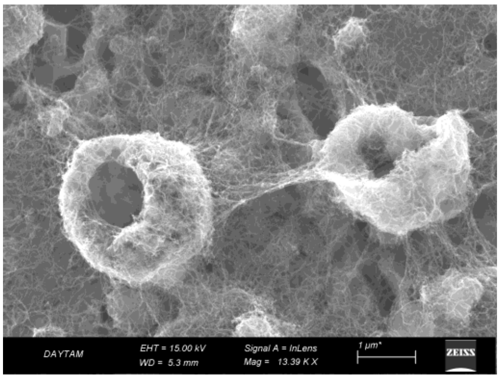

Figure 2. SEM images of Cu/CuONP/MWCNT composite film

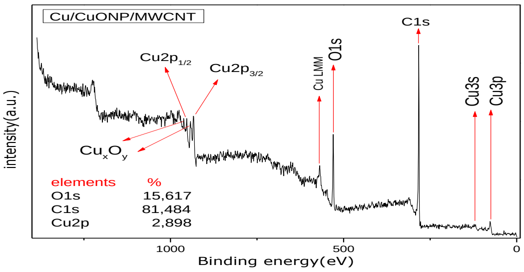

Figure 3. XPS survey spectrum of Cu/CuONP/MWCNT composite film

Development of reactive biohybrid-sensor-systems for the detection of environmentally relevant resources and pollutants in aqueous systems

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The aim of the project is to develop a sensor-system utilizing S-layer proteins to detect analytes with special industrial interest, e.g. copper and rare earth elements and aqueous environments.

Surface layer (S-layer) are the outermost structure in many bacteria and archaea species. They contain of subunits of identical (glyco-) proteins, which can self-assemble to form a highly-ordered crystalline structure of varying symmetry. After extraction from cultivated cells isolated S-layers can be used for a broad range of nanotechnology applications [1]. Furthermore, studies have shown different binding capacities for metal-ions for different S-layers [2]. This together with the possibility to self-assemble on different surfaces leads to the possible development of varying specific sensor-systems.

For this use two sensor-platforms are investigated. The first is a colorimetric-based system using gold nanoparticles (AuNP) functionalized with S-layer proteins [3]. The specific binding properties of the S-layers lead to an aggregation of the AuNP when in contact with the detectable analyte (Figure 1). This is visible as a color-shift and can be measured by UV-vis spectroscopy. Using different s-layer proteins for the functionalization a sensor-array can be developed to detect different analytes.

The second sensor system uses surface-plasmon-resonance (SPR) to self-assemble S-layer on a gold surface and detect the binding of the analytes to the protein layer (Figure 2). Using a broad range of s-layer proteins leads to a sensor array for the specific detection of analytes.

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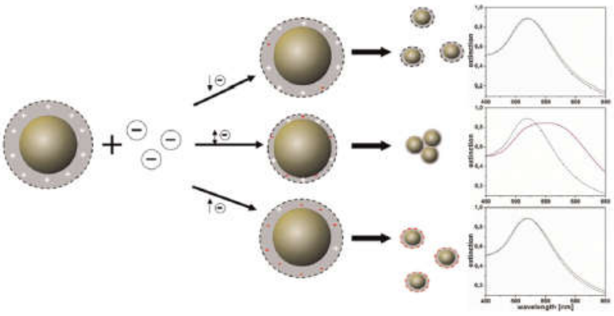

Figure 1. Interaction modes of S-layer functionalized AuNP for different concentrations of the analyte (from Lakatos et al. 2015).

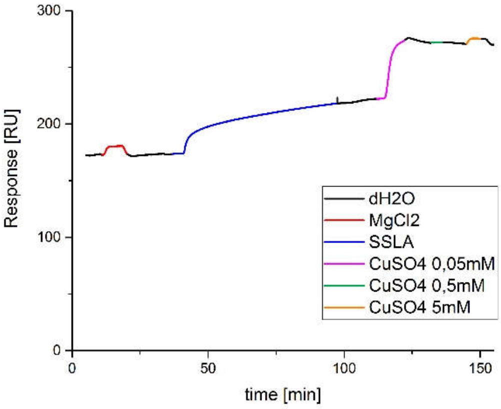

Figure 2. SPR-measurement of the binding of isolated *SslA* protein on gold and the interaction with CuSO4 in increasing concentrations.

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SERS of isotopically labelled $^{12}C/^{13}C$ graphene bilayer: graphene layer as spacer and probe

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Graphene is envisaged to improve significantly the substrates for surface-enhanced Raman scattering of planar aromatic molecules as it can ensure a more even enhancement at different places of the substrate. For this purpose, the role of graphene as a spacer in such SERS platforms has to be addressed. Here, we prepared and probed by Raman spectroscopy hybrid systems constituted by $^{13}C/^{12}C$ bilayer graphene covered by nanostructured gold. Hybrids with both the ^{13}C over ^{12}C layers and in the flipped geometry, and with both the turbostratic and the A-B stacked order have been investigated, and qualitative as well as quantitative information about the enhancement experienced by phonons of the individual graphene layers by the electromagnetic mechanism of SERS were addressed. Here, the top layer of the isotopically labeled bilayer graphene represents the graphene spacer, while the bottom layer mimics a monolayer of target planar aromatic molecules. Both the calculation and the experiment based chiefly on comparison of the relative intensity ratio of the clearly distinguished ^{13}C layer and ^{12}C layer G mode bands jointly indicate that the enhancement of Raman scattering of the molecular monolayer on graphene spacer by the electromagnetic mechanism of SERS will be only 0.7 times lower than that of a monolayer located directly on the nanostructured Au surface

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Development of Printable Composite Metal Ink Based on In-Bi-Sn Ternary Eutectic Alloy for Functional Electronics via Liquid Metal 3D printing

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Liquid metal 3D printing is a promising technology in metal additive manufacturing application such as 3D printed electronics [1]. Field's metal, known as an In-Bi-Sn ternary eutectic alloy, has characteristics of low melting temperature, relatively low resistivity, and low reactivity with air and water below 373K [2] and therefore it is a good candidate material to pattern electrical routes of 3D printed electronics. To enhance the printability of the direct writing of liquid phase of metal, the composite metal was fabricated based on melted In-Bi-Sn eutectic alloy by introducing copper micro flakes as shown in Figure1. In this study, the comparative studies of the Field's metal and the fabricated In-Bi-Sn composite metal were performed and the modified thermodynamic, electrical, and rheological behaviors were analyzed. Due to the additives, the liquidus and solidus temperatures were shifted. Even though non-Newtonian fluidic behavior was enhanced, the conductivity and viscosity of the specimen were increased favorably for printing at 15 wt.% Cu flake.

A functional electronics was designed and developed by liquid metal 3D printing using the fabricated composite metal on the PLA substrate prepared by fused deposition modeling (FDM) additive manufacturing. The simple antenna pattern was successfully printed and demonstrated with a nozzle size of 300µm and a line pitch of 0.5mm and the patterned antenna was provided in Figure2.

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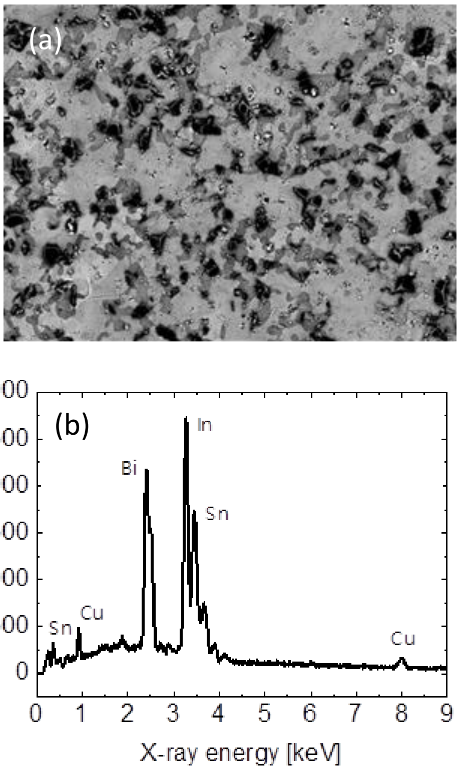

Figure 1. (a) SEM image of composite metal mixture of In-Bi-Sn eutectic alloy and copper micro flake. Note eutectic grain (light grey), Sn rich phase (dark grey), and Cu flake (black) (b) Compositional distribution by EDS analysis

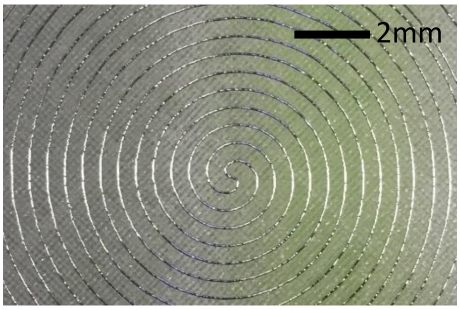

Figure 2. Printed antenna pattern on PLA substrate

Imaging the electronic structure of long acenes generated on-surface

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We present the fabrication of acenes (polycyclic hydrocarbons formed by the linear fusion of several benzene rings) on metallic surfaces. Here, on-surface reduction of specifically designed precursors pushes the boundaries set by stability and allows single molecule investigations beyond pentacene. In particular, scanning tunneling microscopy and spectroscopy of single hexacene molecules is performed to directly visualize the frontier orbital resonances and to capture their narrow energy gap [1]. Due to the high reactivity of hexacene under ambient conditions, scanning probe investigations at the single molecule level could not be obtained so far. In this work, we proof the scalability of a recently introduced on-surface reaction [2] to generate and stabilize long acenes directly on Au(111) by making use of oxygen-containing precursors (see Figure 1). In the last part of this contribution, we analyze the electronic resonances of hexacene and beyond on Au(111) as function of the length.

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Figures

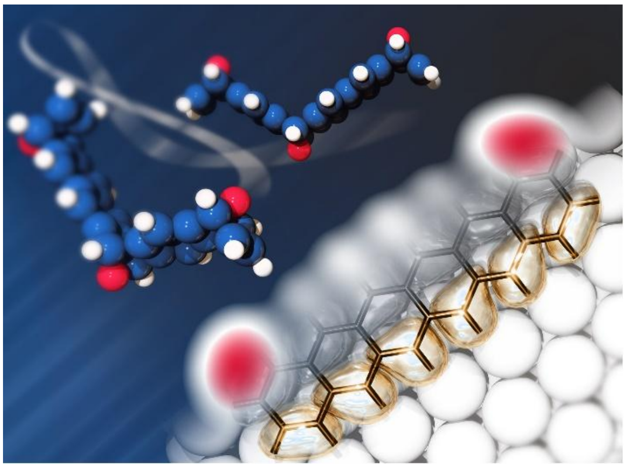

Figure 1. On-surface reduction of air-stable precursors allows the single-molecule investigations of hexacene.

Contrast Agents for MR Imaging: Enhanced T_2 Relaxivity of Zn-Doped Maghemite-Magnetite Nanoparticles

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The effect of Zn-doping into originally spinel structure of Fe_3O_4 on stoichiometry, ^{57}Fe hyperfine parameters and magnetic response is investigated by means of liquid-helium temperature in-field Mössbauer spectroscopy (up to 6 Tesla) and temperature-dependent SQUID magnetometry. While for bulk material, Zn atoms preferably occupy tetrahedral (A) positions, the situation in nanocrystals may differ in dependence on their diameter as well as the method of preparation. Distribution of non-magnetic Zn cations within the tetrahedral (A) and octahedral [B] sites significantly influences the predominant A-B magnetic interactions, causing the change in magnetic structure.

The nanoparticles (NPs) of $Zn_xFe_{3-x}O_4$ with x being 0, 0.05 and 0.36 as determined by X-ray fluorescence spectroscopy, are synthetized by controlled two-step thermal decomposition [1]. The particles' morphology and size distribution as observed via transmission electron microscopy corresponds well to the log-normal distribution. Mean diameters and polydispersity indices are d_0=11.3 nm and σ=0.39 for x=0; d_0=10.6 nm and σ=0.19 for x=0.05; NPs with x=0.33 have bimodal distribution with d_{01}=5.1 nm and σ_1=0.15 and d_{02}=14.4 nm and σ_2=0.06, respectively. The spinel structure is confirmed by X-ray diffraction.

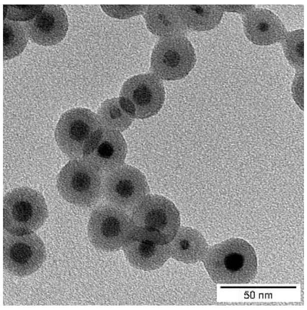

Figure 1. Representative TEM bright field image of $Zn_{0.36}Fe_{2.64}O_4$@SiO_2 NPs with 8.8(8)nm wide shell layer.

The subsequent coating of $Zn_{0.36}Fe_{2.64}O_4$ magnetic cores by silica shell of varying thickness provides colloidally stable particles whose transverse relaxivity (r_2) is analyzed with respect to the applied magnetic field in the range from 0.5 to 11.75 T. The iron concentration (resp. magnetically active atoms) in aqueous suspensions is accurately determined by atomic absorption spectroscopy. The highest observed r_2 value of about 324 Fe $mM^{-1}s^{-1}$ is relatively higher than those previously reported for undoped magnetite NPs [2].

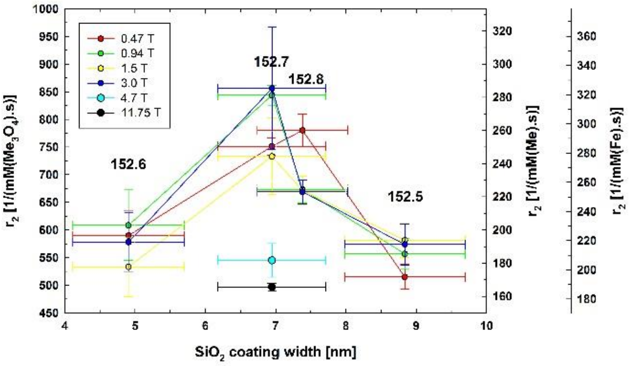

Figure 2. Transversal relaxivity r_2 of $Zn_{0.36}Fe_{2.64}O_4$@SiO_2 NPs versus silica coating thickness for different external magnetic fields, *Me* stands for all metallic atoms in the structure. Connecting lines are only guide for the eye.

The financial support under the grant GAČR 16-04340S is gratefully acknowledged.

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Synaptic devices implemented in two-dimensional layered single crystal chromium thiophosphate ($CrPS_4$).

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The development of reliable memristor devices capable of storing multiple states of information has opened up new applications as neuromorphic computing[1,2]. Recently, Reported ion migration based synaptic memristor devices using two-dimensional (2D) layered transition metal dichalcogenides (TMDs) materials such as MoS_2 and WS_2. Native oxidized layer of sub nanometer thickness exhibits excellent synaptic plasticity and learning capacity close to the ~100mV level of neuron spike by electrically induced oxygen vacancy conductive bridge.[3] However, these devices has dimension limit as reducibility total thickness due to Native oxidized MoO_x/MoS_2 and WO_x/WS_2 heterostructure.

In this work, we fabricated memristor devices of M/I/M capacitor structures using 2D layered $CrPS_4$ single crystal electrolyte. It is used insulator part as electrolyte with controlled difference thickness by mechanical exfoliation method. We observed current-voltage (*I-V*) curves of bipolar resistive switching (RS) behaviors which occurred at low switching voltage with high on/off ratio. Furthermore, we demonstrated in our device including cation movements with multiple resistance states are controlled through repeated stimulation.

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Figures

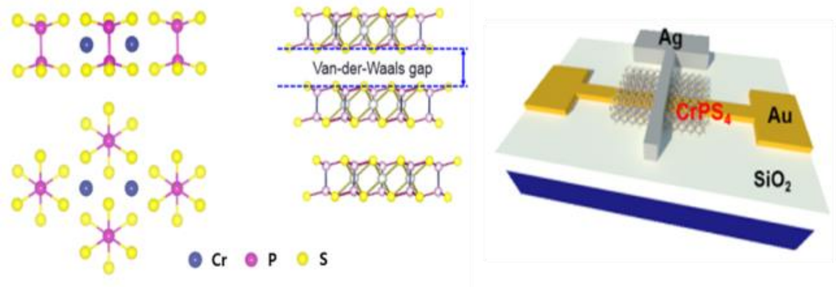

Figure 1. Schematic image of memristor device and 2d layered structure of $CrPS_4$.

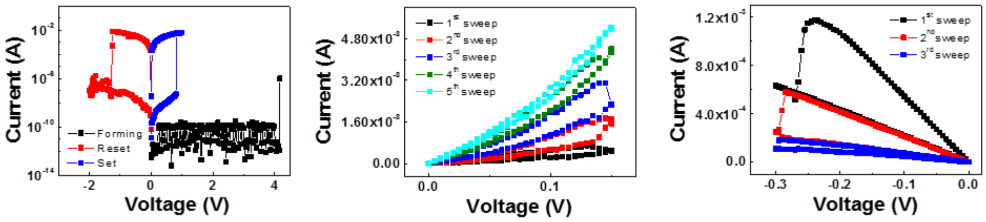

Figure 2. Resistive switching behaviors of memristor devoce.

Obtaining of gold nanoparticles in presence of chitosan. A process thermally assisted

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In recent years, metal nanoparticles have been the subject of many studies. Nanoparticles composed of noble metals, particularly gold, are exceptional due to their special properties, e.g., optical, magnetic, electronic and optoelectronic properties. Polymers have been broadly used to develop metallic nanoparticles taking advantage of their capabilities, either, as stabilizers or simultaneously as reductants and stabilizers. [1,2]

In this work, we show the results of a simple method for obtaining gold nanoparticles in presence of chitosan. The synthesis was developed by thermal assistance, in pyrolysis reactors and in small crucibles during the essays of thermal analysis.

The study include thermal analysis TGA and DSC. The obtained nanoparticles were characterized by UV-Vis spectroscopy, transmission and scanning electron microscopy TEM and SEM.

Acknowledgement

The authors thank FONDECYT projects 1120119 and 1161159 for the partial financial support of this study.

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Figures

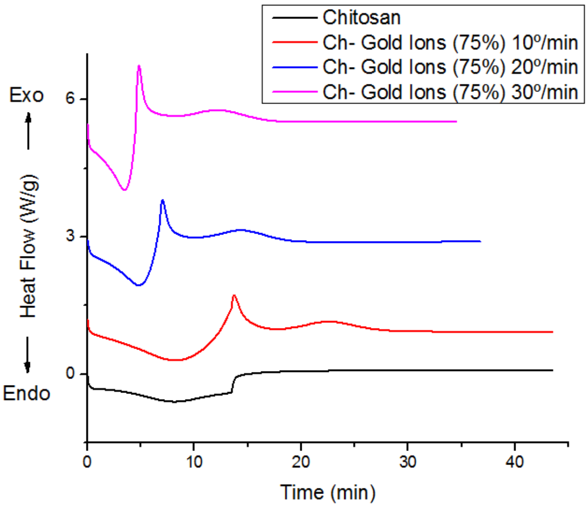

Figure 1. DSC thermograms of chitosan and chitosan with Au III.

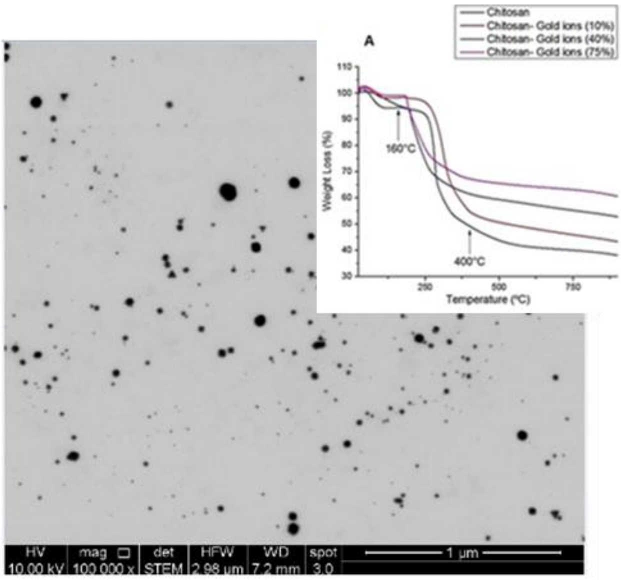

Figure 2. TEM image of gold nanoparticles obtained by chitosan/Au(III) blend heating, and thermal degradation profiles of chitosan/Au(III) blends (insert).

Doped Single-Walled Carbon Nanotubes for Flexible Thermoelectric Applications

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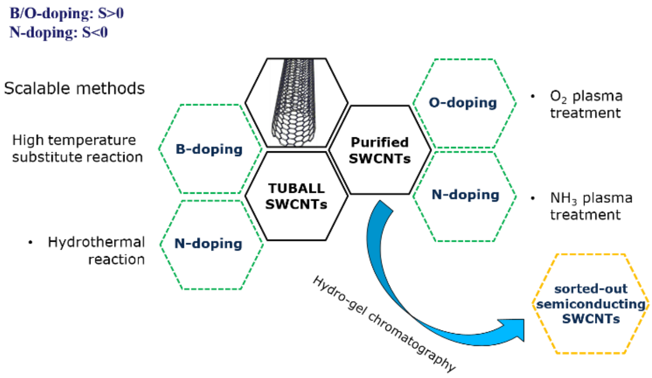
Single walled carbon nanotubes (SWCNTs) have a high potential as flexible thermoelectric (TE) materials owing to their high charge carrier mobility, light weight and outstanding mechanical properties [1]. Recently, purified semiconducting SWCNT films showed TE properties comparable to commercial Bi_2Te_3 alloys [2]. Doping is a crucial step towards TE application of SWCNTs, not only for maximizing their thermoelectric power factor (S2σ), but also for providing n-type nanotubes that are demanded for TE devices (pristine SWCNTs are p-type materials due to oxygen/water absorption). Here doping as well as ambient effects on the TE properties of SWCNTs are investigated. We performed post-synthesis large-scale boron (B-) and nitrogen (N-) doping for commercial unsorted SWCNTs, by high temperature substitutional reaction and hydrothermal reaction, respectively. The maximum achieved dopants concentration were 0.5 at.% for substituting B atoms and 0.4 at.% for quaternary N atoms for B-SWCNT and N-SWCNT samples, respectively. By boron doping, we were able to enlarge both electrical conductivity (up to 250000 S/m) and Seebeck coefficient (up to 30 µV/K) of pristine SWCNTs that ended up at the increase of the power factor to ca. 120 $\mu W/mK^2$. On the other hand, a high amount of oxygen absorbed on N-doped SWCNTs is found to be the main obstacle for achieving negative Seebeck coefficient in ambient conditions.

As an alternative route towards improving TE properties of carbon nanotubes, semiconducting (sc-) SWCNTs were sorted out by gel chromatography, and thin sc-SWCNT films were prepared. By separating semiconducting-only nanotubes, Seebeck coefficient of SWCNT samples has been dramatically increased up to 120 µV/K. Then, the sc-SWCNT films were doped by oxygen or ammonia plasma treatment. The treatment with oxygen plasma caused further increase of Seebeck coefficient up to 160µV/K. Ammonia plasma treatment led to a noticeably higher nitrogen-to-oxygen ratio in sc-SWCNTs than in case of the hydrothermal treatment. The films of N-doped sc-SWCNTs are n-type semiconductors with extremely low negative Seebeck coefficient.



Thus, doping of SWCNTs, especially in combination with sorting-out of sc-SWCNTs, leads to a dramatic enhancement of TE properties of carbon nanotubes. It can be expected, that hybrid composites made of doped SWCNTs and polymers may provide a new avenues for the development of optimal materials for flexible TE applications.

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Computational study of building blocks of 2D polymers confined on the surface of water

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Since the discovery of graphene, two-dimensional materials (2DMs) have become a primary target to study. A promising route in the synthesis of novel 2DMs is given by forming conjugated 2D polymers (2DPs) based on organic building-blocks (monomers) at an air/water interface through the Langmuir-Blodgett method [1]. It is important for the design of the 2DPs to understand the "adsorption" process of the monomers at the water surface and to control their structure on an atomic scale [2].

This work presents a computational study of two different molecules (polycyclic aromatic hydrocarbons) as suitable building blocks for 2DPs using classical Molecular Dynamics (MD) simulations and Density Functional Tight Binding (DFTB) calculations. The MD simulations reveal the preference of the monomers to stay at the air/water surface (Figure 1). Umbrella sampling simulations were conducted to obtain the potential mean force of pulling the molecule out from the water. The latter calculations show an energy minimum at the air/water interface, which is on the order of *-24* kJ/mol. Using the stable monomer geometries from the MD simulations, the formation of dimers at the air/water interface was investigated using the DFTB approach. It is found that the interface stabilizes a flat conformation of the dimer (Figure 2). Constructing ring geometries from the dimers we find different candidates for unit cells, which can realize crystals of the target 2DP. Finally, the stability and electronic structure of the crystals is investigated.

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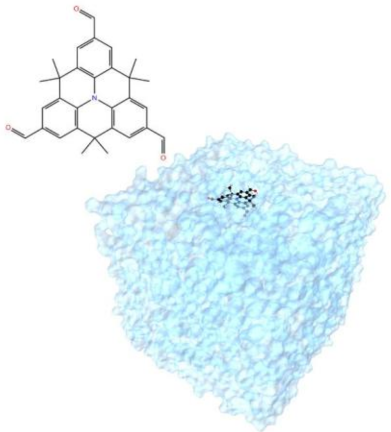

Figure 1. Sketch of the simulation cell consisting of the water slab and the monomer at the vacuum/water interface.

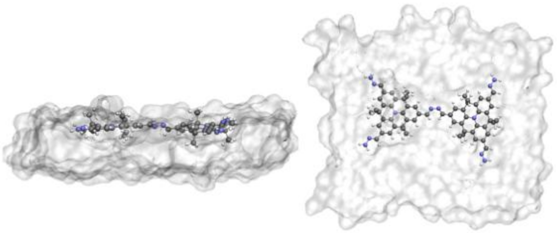

Figure 2. DFTB-MD simulations of the dimer placed on the water surface at *295.15* K.

The performance of few-layer graphene/natural polymer films produced by layer-by-layer

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Abstract

Natural polymers such as chitosan (CHI) and alginate (ALG) are biocompatible materials suitable for implantable devices, however present weak mechanical properties. Mechanical reinforcement can be enhanced with processing techniques that buildup nanostructure such as layer-by-layer assembly (LbL). In the present work suspensions of functionalized graphene nanoflakes (f-GF) and nanoribbons (f-GNR) were prepared from expanded graphite (EG) and multi-walled carbon nanotubes (MWNTs), respectively. The f-GF and f-GNR were produced by different methods [1,2,3]. The layer-by-layer deposition of f-GF or f-GNR and CHI/ALG was investigated and free standing films were produced. The weight incorporation of f-GF and f-GNR was measured. The films were characterized in terms of morphology, mechanical and electrical properties, swelling in water and cytocompatibility. It was observed that graphene increased the storage modulus and dynamic mechanical response at 1Hz and 37ºC, and decreased the electrical resistivity. Biological assays revealed cytocompatibility towards L929 cells. In conclusion, these new f-GF and f-GNR reinforced free standing films present potential for biomedical applications.

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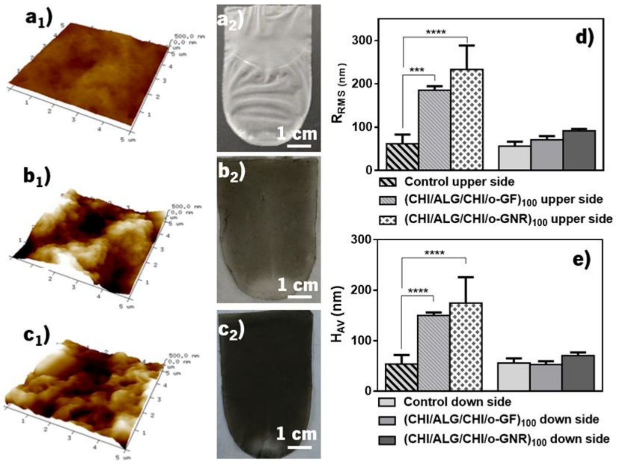

Figure 1. 4 AFM 3D surface images of: a_1-controls FS films, a_2-(CHI/ALG/CHI/o-GF)100 films and c_1- (CHI/ALG/CHI/o-GNR)100 films. (d) RRMS and (e) is the HAV. Photographs of the different films are shown in a_2, b_2 and c_2.

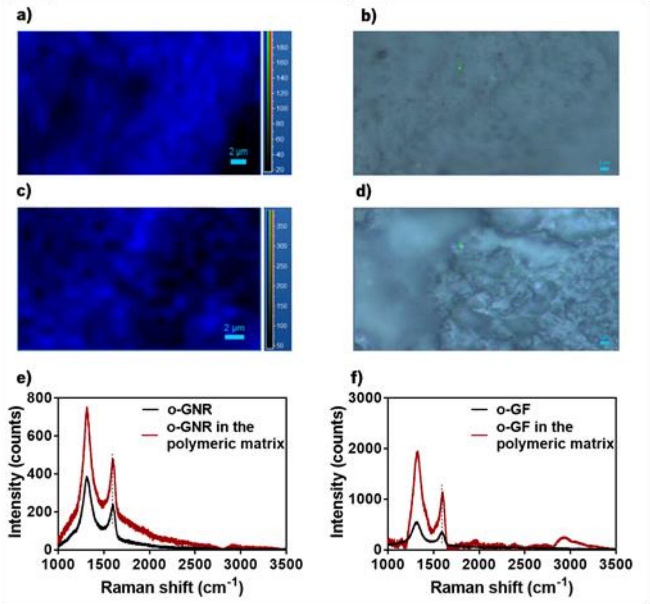

Figure 2. Distribution of o-GNR and o-GF in the CHI/ALG matrix obtained by Raman spectroscopy (a,c); optical image of the o-GNR and o-GF composite films(b,d); Raman spectra obtained for the o-GNR and o-GF before (black line) and after CHI/ALG film production (red line, respectively (e,f).

Highly efficient ammonia sensors based on modified single walled carbon nanotubes

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Carbon nanotubes have emerged as a promising alternative for highly efficient gas sensing technologies due to their remarkable properties like high surface to volume ratios and the possibility of doping or functionalization according to a specific application[1]. In this work, the fabrication and response of gas sensing devices based on networks of single walled semiconducting, pristine (unsorted), boron doped and nitrogen doped carbon nanotubes to low concentrations of ammonia at room temperature was investigated. The chemiresistor-type sensors were fabricated using UV-lithography process, and the nanotubes were deposited using a drop casting approach (Fig. 1) followed by electrical and scanning electron microscopy characterization. Then, the sensors were exposed to 1.5, 2.5, 5, 10 and 20 ppm of NH_3, and the change of current at a fixed voltage as the reaction to the gas exposure was measured.

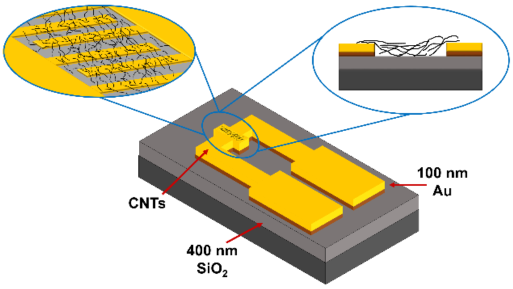

Figure 1. Schematic view of the CNT-based gas sensing device with interdigitated electrodes and SWCNTs on Si/SiO_2 substrate.

The comparison of the detection performance of different devices, in terms of resistance change, combined with the detailed analysis of chemical bonding of dopant atoms to nanotube walls sheds the light on the interaction of NH_3 with CNTs.
Electrical characterization and analysis of the structure of fabricated devices showed a close relation between the amount and quality of distribution of deposited nanotubes and their sensing properties (Fig. 2). Furthermore, sensors based on semiconducting CNTs exhibited the highest sensing responses to all ammonia concentrations compared to other nanotubes. These sensors have 3.5% response to 1.5 ppm of ammonia at room temperature, are able to detect NH_3 at sub-ppm concentrations, and consume only 0.6 µW of power. All this suggest application of these sensors for diagnosis of certain diseases based on the analysis of exhaled breath samples as well as for mobile applications or a remote environment monitoring.

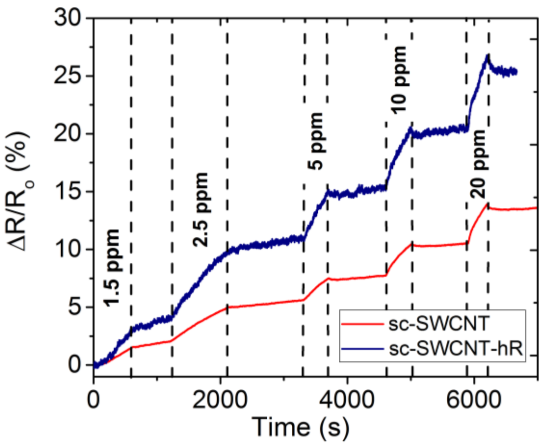

Figure 2. Sensing response $\Delta R/R_0$ of two devices based on semiconducting SWCNTs with different amount of nanotubes under exposure to five different ammonia concentrations. The devices had initial resistance of 268Ω (more nanotubes, red) and 15 kΩ (less nanotubes, blue).

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Surface analysis of Gradient Stainless Steel Buffer Layer to Support Aluminium Nitride Diffusion Barrier for Carbon Nanotubes Growth

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Abstract

To obtain carbon nanotubes (CNTs) by chemical vapor deposition on conductive substrates, such as cooper or stainless-steel, diffusion barriers (DB) are generally used to avoid catalyst diffusion. Two properties of the DB must be thermal stability and expansion coefficient similar to the substrate. Our research is focused on testing a new multilayer with suitable characteristics having an efficient DB functionality. Using DC-pulsed sputtering process we can deposit different combinations of layers on stainless-steel 304 (SS304). In previous works, we used Ti and Ni between SS304 and DB (Al_2O_3 or AlN) to act like a buffer layer, but it requires the exchange of sputtering targets during the deposition process. The multilayer system used in the present work simplify the process by using a target of SS304. The obtained layer was nitrided more and more during deposition. This allows finally to obtain a gradient layer of nitrided steel that acts as a buffer layer for the diffusion barrier of aluminium nitride (AlN). We tested a gradient layer formed by three layers. Each layer is deposited using the same pressure (1 Pa), power (50 W) and frequency (100 kHz, duty-cycle 2016 ns). But the N_2/Ar flow ratio was changed during the deposition process. The initial flow ratio was 0/20 sccm, then was increased to 3/17 sccm and finally was 7/13 sccm. For this study, the three layers were deposited independently on three polished glass substrates during 600 s. X-ray photoelectron spectroscopy (XPS) analysis provided us the chemical composition of each layer forming the gradient stainless steel buffer layer. Rich phases of nitrogen were obtained when the N_2/Ar flow ratio was increased. As expected, gradual nitriding of the stainless steel was shown. Additionally, the distribution of the nitrogen bound to the different elements present in the steel was evidenced. Finally, it was observed that when the N_2/Ar flow ratio increases, the deposition rate of the stainless-steel layers decreases.

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Figures

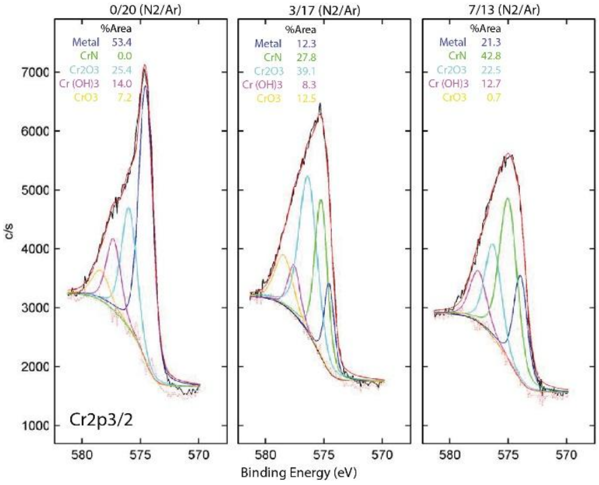

Figure 1. Sample of XPS spectrum $Cr_2p3/2$ detected for the stainless-steel layers deposited on glass under different N_2/Ar flow ratio conditions.

Thermoelectric materials: Switching from p- to n-type by addition of PEG to polymer-SWCNT composites

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Thermoelectric generators (TEG), which can convert waste heat directly into electricity, are one type of promising energy harvesting devices. The thermoelectric (TE) effect (also called Seebeck effect) describes an electrical potential (voltage ΔU) induced by a temperature difference (ΔT) between the two sides of a material. High Seebeck coefficient (S), high electrical conductivity (σ) and low thermal conductivity (κ) are favourable for high TE efficiency with high power factor ($PF = \sigma \cdot S^2$).

An efficient TEG requires high performance p-type (positive S) and n-type (negative S) TE materials. To avoid problems coming from different thermal expansion coefficients or corrosion effects of two different materials, it is desired to combine similar p- and n-type materials for device fabrication. An ideal scenario is to apply the same base material, which can be doped both into p-type and n-type.

In this contribution, we show that melt processed p-type polymer/singlewalled carbon nanotube (SWCNT) composites based on polypropylene (PP) could be converted into relative stable n-type by using a processing additive, polyethylene glycol (PEG), during melt mixing.

To generate p-type composites, SWCNTs of the type TUBALL™ from OCSiAl were employed and melt mixed into a PP matrix using a small-scale compounder. The SWCNTs form an electrical conducting network already at very low amounts of ~ 0.1 wt% [1]. The effect of SWCNT content on σ, S, and PF was studied. The maximum S value reached was 63.8 μV/K, resulting in a power factor of 0.26 μW/(m·K^2) [3]. At the further investigated SWCNT concentrations (0.8 wt% and 2 wt%) and a fixed copper oxide (CuO) content of 5 wt%, the PEG (M_n 10,000 g/mol) addition during melt mixing converted the p-type composites into n-type. Values of S up to – 56 μV/K were achieved using 2 wt% SWCNT and 10wt% PEG, resulting in a power factor of 0.078 μW/(m·K^2) [4].

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Figures

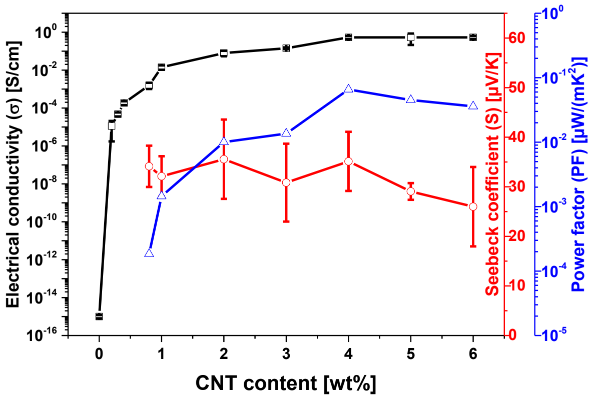

Figure 1. Dependence of TE properties on the SWCNT content for PP based composites [2].

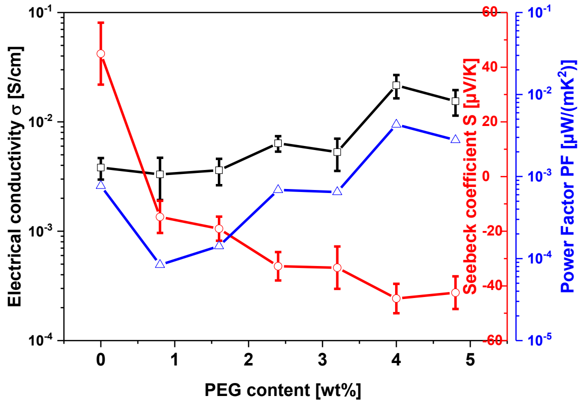

Figure 2. The influence of PEG content on the TE properties for melt mixed composites with fixed SWCNT (0.8 wt%) and CuO (5 wt%) concentration [4].

Light-emitting polymer nanofibers doped by organic and biological chromophores: morphology, waveguiding properties, and energy transfer

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Light-emitting micro- and nanostructures and smart materials based on electrospun fibers are being widely studied and they can find use in the realization of lasers, light-emitting diodes, field-effect transistors, photovoltaic cells, optical sensors and many more [1, 2]. Thanks to their anisotropic geometry, light-emitting fibers have features not achievable in macroscopic scale. In particular, they can produce polarized light-emission, but also amplify self-emitted light signal and guide it along the longitudinal axis of the fibers [2]. The success of such materials is supported by electrospinning, a one-step, simple and low-cost technique that allows flexible and versatile micro- and nanofibers to be realized through the stretching of a polymeric solution by means of an assisted electrical field [3].

A simple method to produce light-emitting fibers consists in electrospinning inert polymers doped by organic chromophores. Generally, small fluorescent molecules are cheap and efficient in providing lasing emission, and they are suitable to realize light-emitting advanced systems with color tunability, especially when used as pairs for Förster Resonant Energy Transfer. In this respect, organic chromophores can be present in aggregated emissive forms and lead to a wide range of tunability [4]. Luminescent proteins [5] can be also processed and embedded into fibers designed to exploit their emissive properties. These molecules were successfully embedded in core-shell fibers by coaxial electrospinning technologies, realizing a suitable micro-environment for preserving their bio-optical functions [6, 7]. Here we present and discuss processing parameters, physical properties and potential applications of light-emitting nanofibers based on small organic dyes and luminescent proteins. The morphology, sub-wavelength guiding of light, as well as energy transfer phenomena are carefully analyzed. Perspectives in the fields of miniaturized optical sensors and organic lasers are especially promising, due to the interplay of waveguiding and emission properties of the hybrid electrospun nanomaterials.

The research leading to these results has received funding from the European Research Council under the European Union's Seventh Framework Programme (FP/2007–2013)/ERC Grant Agreement n. 306357 (ERC Starting Grant "NANO-JETS").

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Real-time in-flow impedance sensing of microparticles using gold nanowires

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Detection of pathogens at low concentrations and sample volumes is one of the mainstreams in the current biomedical research due to the distinct demographic changes and wide spreading of the chronic and severe illnesses. Conventional pathogen detection approaches enzyme-linked immunosorbent assay (ELISA), flow cytometry or DNA amplification using polymerase chain reaction require high effort and time with regard to sample preparation, signal processing and data analysis. Furthermore, since these techniques rely on optical detection, high sample volumes, analyte labeling and bulky equipment is mandatory.

Consequently, there is a high demand for precise, cheap and portable sensor devices for application in the environment where the patient needs a proper treatment without available qualified personnel and hospitals, e.g. in developing countries. In this, the next generation of bio-sensors for the detection of biological species also require high sensitivity and selectivity at high throughput due to low concentration of analytes, *e.g.* pathogens[1], and in complex media like blood or saliva.

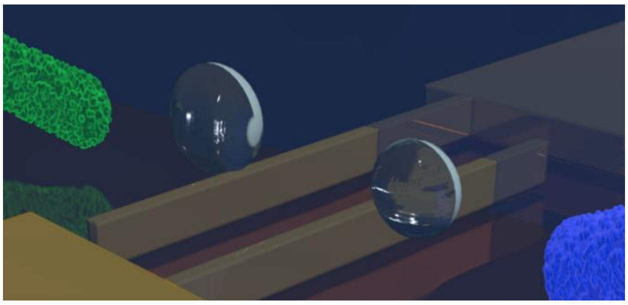

Figure 1: Schematic illustration of the nano capacitor sensing device. The analyte solution is guided between the gold nanowire electrode pair thereby altering the impedance of the sensing structure

We faced the challenge to establish a MEMS-sensor capable of single cell detection based on dynamic impedance analysis using gold nanowires to overcome the aforementioned limitations (see Figure 1). The detection of microparticles one by one is realized in flow, employing the cytometry principle. The transport system consists of a 3D focusing microfluidic structure, which converts the particle solution to interdigitating top-down fabricated gold nanowires, allowing higher sensitivity and selectivity due to electric field enhancement between the nanowires[2] (See Figure 2). We demonstrate the detection of single particles in real-time based on impedance changes in a proof-of-principle approach.

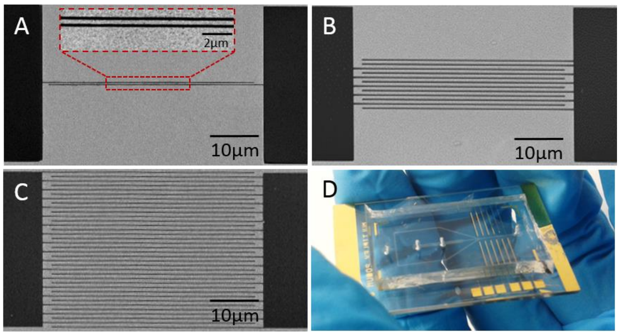

Figure 2: Geometries of the sensing structures with increasing sensing area: (A) Single nanowire pair (B) 12 nanowires pairs resulting in a sensing area of 500µm² (C) 36 nanowires pairs resulting in a sensing area of 2500µm²

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Asymmetry as a key factor for increasing the functionality of a molecular logic gate

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Design and fabrication of nanoscale functional electronic units remains a main task of molecular electronics. Recently, it was shown, that by manipulating single gold atoms under symmetric Y-shaped molecule, one could demonstrate the functionality of a NOR logic gate.[1] In our work, we investigate the role of asymmetry for the functionality of such a system. By applying classical gold inputs in different configurations, we can obtain various logical behavior of the system as an output, measured by the shifts of scanning tunneling spectra. Thus, bringing the asymmetry into the molecule increases the functionality of a molecular logic gate. To fabricate a fully conjugated asymmetric Y-shaped molecule on Au(111) surface, we employ surface-assisted cyclodehydrogenation.

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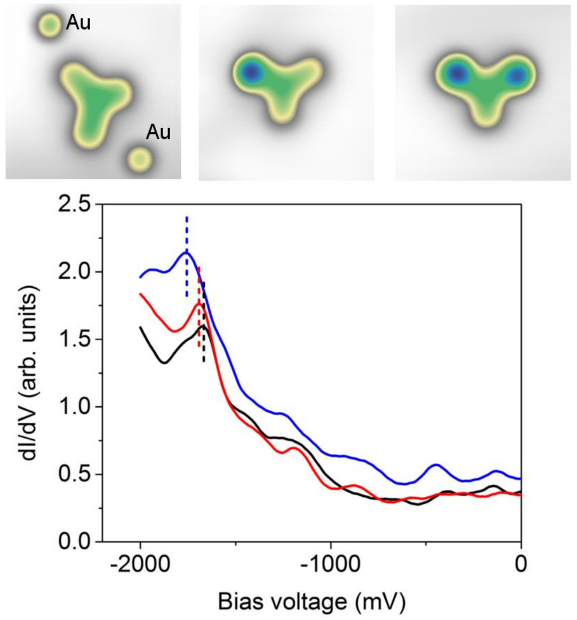

Figure 1. Demonstration of NAND molecular logic gate by successively bringing Au atoms under the longer branches of an asymmetric Y-shaped molecule.

Coordination Polymer Framework-Based On-Chip Micro-Supercapacitors with AC Line-Filtering Performance

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On-chip micro-supercapacitors (MSCs) are important Si-compatible power source backups for miniaturized electronics, owing to their rapid energy-harvesting features, burst-mode power delivery, and in particular the good compatibility with Si. However, current on-chip MSCs require harsh processing conditions (high-temperature fabrication, oxygen plasma and wet-chemistry etching, etc.), and typically perform like resistors when filtering ripples from alternating current (AC). Therefore, the development of Si-compatible MSCs with facile fabrication procedure is an urgent task for their practical applications.

In this work, we demonstrated the first on-chip MSC based on a coordination polymer framework (PiCBA) by using a facile layer-by-layer strategy. Owing to the good carrier mobility (5×10^{-3} $cm^2 \cdot V^{-1} \cdot s^{-1}$) of PiCBA, strong interaction between PiCBA and patterned Au current collectors, and in-plane geometry, the as-fabricated MSCs delivered high specific capacitances of up to 34.1 $F \cdot cm^{-3}$ at 50 $mV \cdot s^{-1}$, a volumetric power density of 1323 $W \cdot cm^{-3}$ and an energy density of 4.7 $mWh \cdot cm^{-3}$. Moreover, the fabricated MSCs exhibited typical AC line-filtering performance (−73° at 120 Hz) with a short resistance-capacitance constant of ~0.83 ms, which is well comparable to the state-of-art MSCs. This study not only provides a general, easy method for the preparation of on-chip MSCs, but also demonstrates the remarkable energy storage potential of coordination polymer frameworks.

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Figures

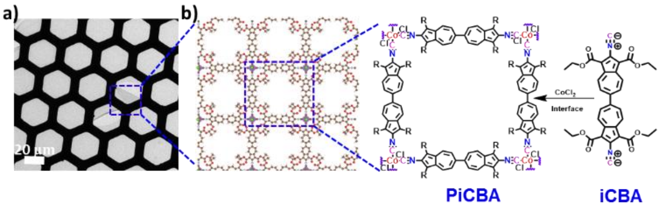

Figure 1. a) Uniform and free-standing PiCBA monolayer film; b) Synthesis of PiCBA film through the coordination reaction between isocyanide and cobalt ions.

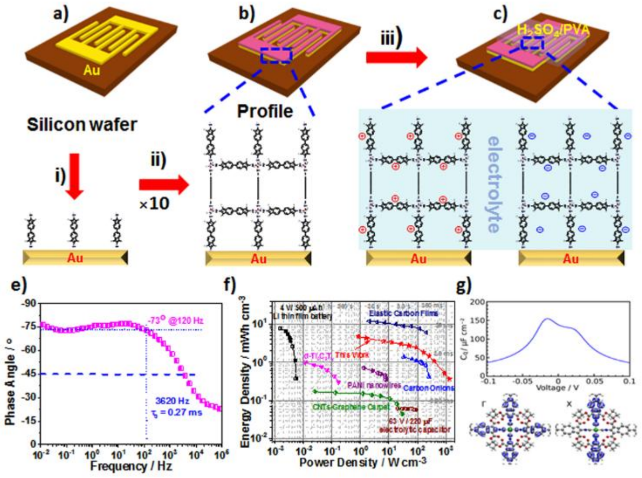

Figure 2. a-c) Schematic illustration of LBL fabrication of PiCBA films on Au interdigital electrodes; e) Impedance phase angle on the frequency for the PiCBA-based microdevices; f) Ragone plots for PiCBA; g) Calculated quantum capacitance.

Synaptic plasticity and learning in ferroelectric tunnel junction

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In neuromorphic computing, synapse plays the key of role by varying its connection weight between two neurons, which is known as synaptic plasticity. Among many different candidates for synaptic devices, two-terminal ferroelectric tunnel junction (FTJ) has demonstrated that gradual switching between on-state and off-state induced by DC voltage pulses strongly depend on their amplitude, duration or number, which simultaneously control ferroelectric domain configurations. However, its limited barrier height modulation inevitably gives rise to low on/off ratio. Here, we report a synaptic metal/ferroelectric /metal device which shows a giant on/off ratio (~10^7). The device also shows synaptic plasticity, learning and memory function by the modulation of tunneling barrier width. Its excellent performances may result from combination of ferroelectric polarization and migrated ions.

Figures

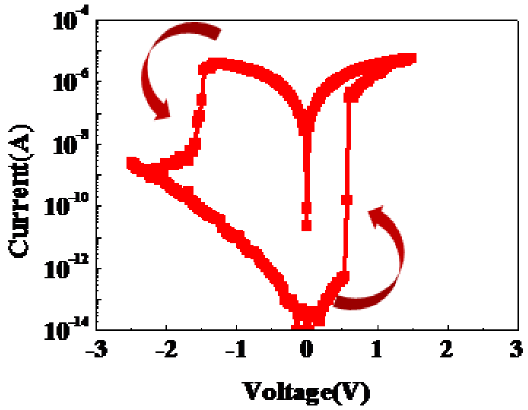

Figure 1. Resistive switching behavior.

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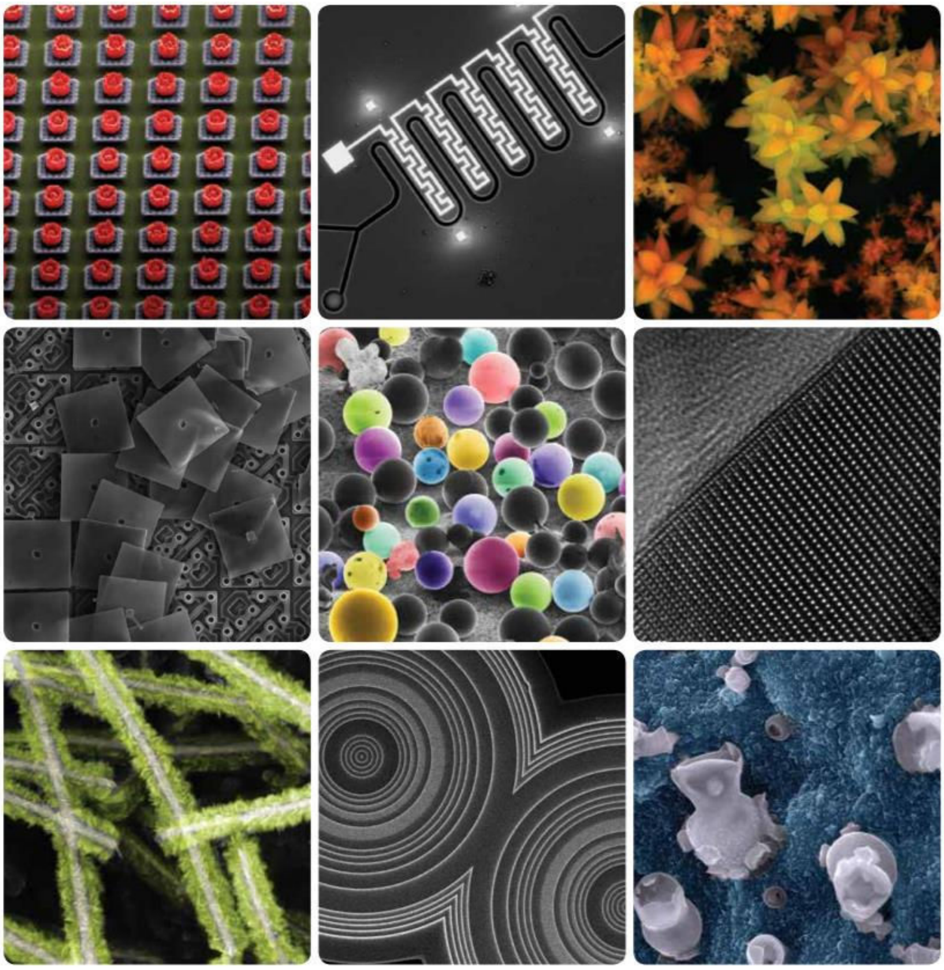

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