Nano-M&D 2019

"Fabrication, Properties, and Applications of Nano-Materials and Nano-Devices"

International Conference

Abstract Book

Savoy Beach Hotel, Paestum, Salerno (Italy)

June 04-08, 2019

INTRODUCTION

The International Conference Nano-M&D 2019 *"Fabrication, Properties, and Applications of Nano-Materials and Nano-Devices"* brings together experts in the field of *Nano-Materials and Nano-Devices* in the ancient city of Paestum, UNESCO site.

The Conference is organized by the Physics Department of the University of Salerno and by the International Institute for Advanced Scientific Studies "E.R. Caianiello", under the Patronage of the Superconductors, Innovative Materials and Devices (SPIN) Institute of the Italian National Research Council (CNR) and Confindustria Salerno.

The Conference programme is scheduled in oral and poster presentations, with the aim of stimulating discussions and knowledge exchange in the following areas:

A) Fabrication, Properties, and Applications of
- A.1. *2D Materials (MoS_2, hBN, etc)*
- A.2. *Carbon Materials: Graphene, CNTs, Nanodiamond,...*
- A.3. *Semiconductors (III-V, Oxides, Organic,…)*
- A.4. *Nanowires*
- A.5. *Nanosensors*
- A.6. *Quantum dots*
- A.7. *Nanomagnetics*
- A.8. *Topological Insulators*

B) Nano-Electronic Devices
- B.1. *Nanoelectronics (FETs, information storage devices, RF passive devices)*
- B.2. *Sensors*
- B.3. *Spintronics*
- B.4. *MEMS/NEMS*
- B.5. *Energy harvesting and storage*
- B.6. *Nano-Biomedicine and bio-devices*
- B.7. *Hardware Realisation of Neuromorphic Functions*

C) Chemistry of 2D Materials
- C.1. *Bottom-up growth*
- C.2. *Synthesis, processing and characterization*
- C.3. *Functionalization*
- C.4. *Synthetic materials*
- C.5. *Design of 3D functional materials*
- C.6. *Composites, foams, coatings, and membranes*
- C.7. *Electro- and Photo-catalysis*

The social events include a visit to the Paestum Archeological site and the National Museum-Guided tour on 6th June afternoon and a Social Dinner on 7th June, and encourage scientific discussions in a relaxed atmosphere.

We wish you a wonderful stay at the Nano-M&D 2019 International Conference.

Antonio Di Bartolomeo
Filippo Giubileo
Chairs

The event is organized by

UNIVERSITÀ DEGLI STUDI DI SALERNO
Dipartimento di Fisica E.R. Caianiello

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INVITED SPEAKERS

ABATE Antonio - *University of Napoli, Italy*

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CAMILLI Luca - *DTU, Denmark*

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HE Jianying - *Norwegian University of Science and Technology, Norway*

HURLEY Paul - *University College Cork, Ireland*

IANNAZZO Daniela - *University of Messina, Italy*

JESSEN Bjarke S - *Technical University of Denmark, Denmark*

JIANG Kaili - *Tsinghua University, Beijing, China*

JOYCE Hannah - *University of Cambridge, UK*

KELLICI Suela - *London South Bank University, United Kingdom*

KONDO Hiroki - *Meijo University, Japan*

KOTAKOSKI Jani - *University of Vienna, Austria*

LEE Hu-Jong - *Pohang University, Republic of Korea*

LISCIO Andrea - *IMM-CNR, Italy*

MACAGNANO Antonella - *IIA-CNR,Italy*

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VENUE

The Conference will be held at the Savoy Beach Hotel in Paestum, Italy.

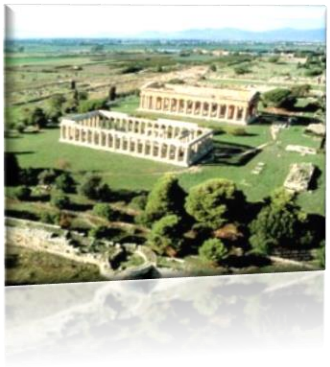
Savoy Beach Hotel Paestum is a 4 Star Luxury Hotel and Congress Site. In the wonderful Cilento, a few steps from the sea, this exclusive hotel in Paestum is equipped with everything you want to make your stay unforgettable. Private beach, swimming pool, tennis courts, fine dining restaurant, Privilege rooms and suites that combine contemporary elegance to the timeless charm of Vietri ceramics. Located in one of the most beautiful areas of Campania, it allows easy access to the bustling Salerno and the most iconic towns such as Acciaroli, Castellabate and Agropoli.

SOCIAL EVENTS

Excursion on Thursday, 6th June (afternoon)

Visit to the Archaeological Site and the National Museum-Guided tour

Paestum is a city of ancient foundation. It was born with the name of Poseidonia in the 6th century BC, built by the Achaeans, Greek colonists from Sibari who chose it as a maritime commercial centre.Tourist resort, Paestum is nowadays at the same time one of the most important archeological centre in Italy and a well-known seaside resort, with its large beach, lined with pine wood and rich of hotels and outdoor facilities. Entering the ancient city is like engaging in an extraordinary journey through time, for the indescribable charm possessed by the well kept monumental structures. The wall around the ancient town is one of the most important examples of town fortification from the Western Greek period. The group of temples, all close to each other, is also very impressive. The largest one is Poseidon's, built in 450 BC, considered by scholars the greatestexample of Doric temple architecture, with its magnificent triangular frontons and the remains of two altars used for the sacrifices to goddess Hera Argiva. The most ancient temple is the so-called Basilica, of the 6th century BC, dedicated to Hera, of which 50 original Doric columns remain intact, the sacred well and the sacrificial altar. Then there is Cerere's temple, dedicated to Athena, with 34 fluted columns. The area is crossed by the Holy Road, along which many important civil and religiuous settlements have been found.You also ought to visit the National Archaeological Museum, where there are sculptures, bas-reliefs and tools from the excavation. Here you can also see the famous “Tuffatore”, recovered from a Greek tomb.

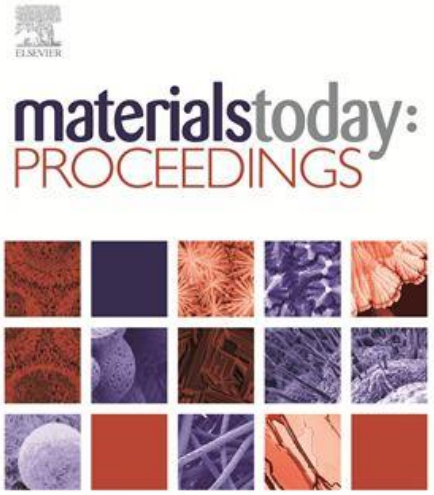


Social Dinner on Friday, 7th June

The social dinner will be held at the Hotel Savoy Beach in Paestum

PROCEEDINGS

Participants at Nano-M&D 2019 International Conference can submit papers for publication in



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Deadline for submission: June 30th, 2019

The manuscripts can be loosely related to the Conference presentations.

International Conference Nano-M&D 2019

Scientific Programme

Tuesday, June 4th	
14:20	**Opening**
	Session 1: Nano-Materials for Sensing *(Chair: F. Rossella)*
14:30	Effect of defects and adsorbents on the performance of optoelectronic devices based on atomically thin materials. **Barbara**
14:45	Laser-irradiated 2D materials: a new path towards straintronic devices. **De Sanctis**
15:00	Electronic Detection of Oxygen Adsorption and Size-Specific Doping of Few-Atom Gold Clusters on Graphene. **Van de Vondel**
15:15	Graphene quantum dots as smart nano-carriers for cancer therapy. **Iannazzo**
15:30	Molecularly imprinted nanogels combined to plastic optical fibre: influence of the nanostructure to the sensor response. **Bossi**
15:45	Electrospun nanocomposite nanofibers in chemical sensors for gaseous compounds. **Macagnano**
16:00	Ion imprinting with graphene oxide and its application in electrochemical sensing. **Jaroslav**
16:15	Structural Changes on Supramolecular Organization of Bitumen Induced by Advanced MWCNTs Based on Silica: Physical Chemistry Characterization. **Oliviero Rossi**
16:30	*Coffee Break*
	Session 2: Nanowires *(Chair: P. Barbara)*
17:00	Advanced field effect control of semiconductor nanowire-based devices. **Rossella**
17:15	Towards ultrafast and highly efficient optoelectronic devices based on III–V nanowires. **Joyce**
17:30	Chemical sensing with ZnO nano and microwires. **Baratto**
17:45	Hybrid Nanowire Based Quantum Networks at Atomic Scale: from growth mechanisms to properties. **Arbiol**
18:00	Bottom-up and Top-down Fabrication of GaN Nanowires in Molecular Beam Epitaxy. **Fernandez Garrido**
18:15	Synthesis, characterization and chemical functionalization of germanium nanowires. **Bosi**
Wednesday, June 5th	
	Session 3: 2D Materials Fabrication (I) *(Chair: M. Batzill)*
09:00	Growth and Applications of Hexagonal Boron Nitride. **Shin**
09:15	Recent Advances in the Growth of Transition Metal Dichalcogenides by Thermally Assisted Conversion. **McEvoy**
09:30	Structure and Dynamics of Alkali-Metal Intercalated Black Phosphorus. **Herwig**
09:45	Growth and application of MoTe2, WTe2 and PtTe2 films. **Mc Manus**
10:00	Ge-based layered materials with high anisotropy. **Camilli**
10:15	Intrinsic properties of single layer molybdenum disulfide prepared by different methods. **Pollmann**
10:30	*Coffee Break*
	Session 4: 2D Materials Fabrication (II) *(Chair: H. Peterlik)*
11:00	Graphene-like silicene grown on inert graphite surface. **Scarselli**
11:15	Growth and characterization of TMD heterostructures. **Peters**
11:30	Hierarchical carbon coated 3D-CZTS nano-structural anode material for high performance LIB applications. **Chen K**
11:45	From Liquid to Solid State: highly homogeneous, smooth, and transparent WS2 – polymer films of of Liquid Exfoliated dispersions. **Szydlowska**
12:00	Bio-applications of semiconductor nanowires. **Prinz**
12:15	New Pathways in the Synthesis of 2-Dimensional Materials. **Kellici**
12:30	*Lunch Break*

	Session 5: Energy Generation/Storage *(Chair: Sergio Pagano)*
14:30	Conduction Current and Displacement Current in Electric Generators. **Zhang**
14:45	Perovskite solar cells. **Abate**
15:00	Nanostructured Functional Polymers for Electrical Energy Storage. **Thelakkat**
15:15	VACNT growth on Aluminium: towards innovative supercapacitor nanocomposite electrodes. **Pinault**
15:30	Composite nanostructures for energy harvesting. **Vomiero**
15:45	Nanostructured materials for energy conversion. **Cavaliere**
16:00	Annealing Temperature Grain Size dependence in Room Temperature Sputtered Gadolinium doped Ceria thin films for SOFC applications. **Coppola**
16:15	Electric transport and voltage-noise properties of granular aluminum oxide nanowires. **Barone**
16:30	*Coffee Break*
17:00	***POSTER SESSION***
	Thursday, June 6th
	Session 6: Transport in Composite Materials and Interfaces (I) *(Chair: P. Hurley)*
09:00	Engineering thermal boundary conductance of a metal/polymer interface. **He**
09:15	Transition metal dichalcogenides in back-gate field effect transistors. **Di Bartolomeo**
09:30	Innovative Nano-Materials and Nanoscale Devices for the end of the Roadmap. **Balestra**
09:45	Scanning probe microscopy based fabrication and characterization of sub-micron Schottky junctions on as-grown graphene/Ge(100). **Notargiacomo**
10:00	Electron-transporting perylene diimide films deposited by supersonic molecular beams. **Barra**
10:15	Microwave plasmon resonance in high-mobility hBN-encapsulated graphene. **Mele**
10:30	*Coffee Break*
	Session 7: Transport in Composite Materials and Interfaces (II) *(Chair: J. He)*
11:00	Investigating the Electronic Properties of Oxide/MoS2 Interfaces. **Hurley**
11:15	Mesoscopic Percolating Resistance Network in Reduced Graphene Oxide Thin Film. **Liscio**
11:30	Organic field-effect transistor structures as a truly multifunctional platform: from light-emission to cell interfacing. **Muccini**
11:45	Field-modulated Graphene/Silicon Schottky diodes fabricated in a fully CMOS-compatible process line. **Alvarado**
12:00	Novel two-dimensional material device concepts through multi-scale simulations. **Marian**
12:15	Influence of graphene particles on morphology and patterns on dewetting of thin polystyrene film. **Basu**
12:30	*Lunch Break*
19:00	***EXCURSION***
	Friday, June 7th
	Session 8: Properties and Functionalization of Layered Materials (I) *(Chair: R. Yakimova)*
09:00	Effect of disorder on the magnetic stability of MoS2 nanoribbons with zigzag edges. **Hagymasi**
09:15	Atomic-scale Engineering of 2D Materials. **Kotakoski**
09:30	Introducing Functionalities in van der Waals materials by Lattice Modifications. **Batzill**
09:45	Two-dimensional nanomaterials for artificial photosynthesis: Turning CO2 into a valuable resource. **Chen LC**
10:00	Layer and photoluminescence engineering of Molybdenite. **Ottaviano**
10:15	Defects, interlayer coupling and Fermi resonance in 2D Materials. **Bendiab**
10:30	*Coffee Break*

	Session 9: Properties and Functionalization of Layered Materials (II) *(Chair: L. Ottaviano)*
11:00	Non-Covalent Functionalization of Monolayer MoS2 – Tuning the Electronic Structure. **Siris**
11:15	Lithographic band structure engineering of graphene. **Sorensen Jessen**
11:30	Scattering Theory of Graphene Grain Boundaries. **Romeo**
11:45	Manipulation of epitaxial graphene towards novel 2D materials. **Yakimova**
12:00	Composition and Electronic Properties of PtSe2 and other Transition-Metal Dichalcogenides Investigated by Photoelectron Spectroscopy. **Stimpel-Lindner**
12:15	Spectroscopy of inelastic processes in quantum Hall edge channels: a possible resolution to the missing energy problem. **Meir**
12:30	*Lunch Break*
	Session 10: Quantum Phenomena *(Chair: A. Liscio)*
14:30	Entanglement manipulation in hybrid TI-S nano-devices. **Braggio**
14:45	Strong proximity Josephson coupling in heterojunctions of 2D materials. **Lee**
15:00	Atomic-scale spin dynamics. **McMurtrie**
15:15	Spintronics at the interface. **Zanolli**
15:30	Stability and lifetime of magnetic skyrmions from density functional theory. **Delin**
15:45	Mechanisms of photoconductivity in atomically thin InSe and GaSe. **Frisenda**
16:00	Optical probes of defects in lead halide perovskites. **Barker**
16:15	Bent-Lattice Nanostructure in Crystallized Amorphous Films: from Transrotational Nanoengineering to Novel Amorphous Models. **Kolosov**
16:30	*Coffee Break*
	Session 11: Nano-Materials: Synthesis and Characterization (I) *(Chair: N. McEvoy)*
17:00	Bottom-up synthesis of atomically precise graphene quantum dots. **Narita**
17:15	Self-assembling at molecular resolution: the power of organizing the unorganized. **Posocco**
17:30	Fabrication and characterization of nanomaterial-based sensor devices using solution printing method. **Sugahara**
17:45	Laser ablation synthesis in solution and nanoalloys: a fruitful combination. **Amendola**
18:00	Advances in Properties and Synthesis of MoS2 and WS2 nanotubes. **Zak**
18:15	Nanocrystal dimers: fabrication and properties. **Striccoli**
20:00	***SOCIAL DINNER***
	Saturday, June 8th
	Session 12: Nano-Materials: Synthesis and Characterization (II) *(Chair: A. Narita)*
09:00	Amorphous and crystalline gallium oxide thin films by atomic layer deposition. **Dubourdieu**
09:15	Graphene Technology: synthesis, characterization and reliability-driven technological device integration. **Morandi**
09:30	Preparation of Graphene Oxide- Quantum Dot Hybrids for the Detection of Ascorbic Acid. **Kim**
09:45	Plasma-assisted Synthesis and Modification of Carbon Nanowalls for Emerging Applications. **Kondo**
10:00	The properties (and some applications) of graphene grown at high T on Co. **Amato**
10:15	Electrochemical lithiation of epitaxial graphene for rechargeable batteries. **Shtepliuk**
10:30	*Coffee Break*
	Session 13: Nanotubes and Nanowires *(Chair: A. Di Bartolomeo)*
11:00	Growing Highly Pure Semiconducting Carbon Nanotubes for Nanoelectronics by Electrotwisting the Helicity. **Jiang**
11:15	Application of low-cost MWCNT/polymer based heating elements as room temperature NIR bolometers with high signal to noise ratio. **Neitzert**
11:30	Elasto-mechanical study of MoS_2 domes by Atomic Force Microscopy and Spectroscopy. **Di Giorgio**
11:45	Analysis of zinc ions supersaturation during the growth of ZnO nanorods. **Basinova**
12:00	Functionalization of carbon nanotubes for nitroaromatic explosive detection. **Musayeva**
12:15	**Closing**

LIST OF POSTERS

Name	Surname	Title of POSTER	ID
Zeljko	**Crljen**	Optimized Model for Non-ideal Organic Electrochemical Transistors Impedance	P01
Ana Laura	**Curcio**	Optical Materials Effects produced by Cadium insertion in ZnO	P02
Surangsee	**Dechjarern**	Optimization of wear resistance of knee joint implant made of titanium alloy with coating treatments and UHMWPE reinforced by carbon nanofiller and cryogenic treatment using Taguchi method	P03
Cristina	**Dumitriu**	Nanostructured electrochemical platform used for gluten presence evaluation	P04
Claudio	**Ferrari**	Sensors based on carbon nanotubes and germanium nanowires for explosive detection	P05
Armando	**Galluzzi**	Influence of citric acid and oleic acid coating on the ac magnetic properties of Fe_3O_4 magnetic nanoparticles	P06
Filippo	**Giubileo**	Field Emission Characterization of MoS_2 Nanoflowers	P07
Veronica	**Granata**	Effect of different atmospheres on the synthesis of $Ba_2CuGe_2O_7$ single crystals	P08
Alessandro	**Grillo**	Field-emission properties of β-Ga_2O_3 nanopillars	P09
Richard	**Harris**	Magnetic monodispersed nanoparticles as drug carriers: a simulation and experimental study of Fe_3O_4 and temozolomide with nanometer precision size control.	P10
Tatsiana	**Henarava**	The determination of polycyclic aromatic hydrocarbons content in exhaust gases formed during carbon nanomaterials synthesis	P11
Laura	**Iemmo**	Effect of electron irradiation and field emission from MoS_2	P12
Mariagrazia	**Iuliano**	Ag/GO Nanocatalysts for N-Alkylation	P13
Angela	**Longo**	Optical grade epoxy-metal nanocomposites as encapsulating for diffuse light-emitting diodes	P14
Giuseppe	**Luongo**	The role of the substrate in graphene/Silicon Schottky diode	P15
Enrique	**Miranda**	SPICE Model for the Conduction Characteristics of Hexagonal Boron Nitride-Based Resistive Switching Devices	P16
Andrea	**Notargiacomo**	Nanoscale surface texturing of porous silicon carbide slabs by fs laser and plasma treatments	P17
Cormac	**Ó Coileáin**	Synthesis of Pt based dichalcogenides via thermally assisted conversion	P18
Georgy	**Pakhomov**	Crystallization in Vacuum-Deposited CuI/Cl6Subpc bilayers for Photovoltaic Applications	P19
Mariano	**Palomba**	Graphene nanoplatelets supported by low density polyethylene	P20
Marialilia	**Pea**	Zn nanoparticle formation in FIB irradiated single crystal ZnO	P21
Domenic Prete	**Prete**	Electrolyte gating of substrate-unbound nanowire-based devices	P22
Davide	**Scarpa**	Novel Pt/Ni/NiO based electrodes for electrocatalytic biodiesel production from palm oil	P23
Manuela	**Scarselli**	3D multifunctional carbon nanotube networks	P24
Aleksandra	**Sosna-Glebska**	UV-enhanced silicon detectors with zinc oxide nanoparticles acting as wavelength shifters	P25
Domenico	**Spina**	From waste to biofuel: a new nano-carbo-catalyst	P26
Chih-Wei	**Tsai**	Photoluminescence of Metal (II) Imidazolate complexes (ZIFs) for sensing alcohols	P27
Francesca	**Urban**	A study of the external stimuli on hysteresis and electrical properties of TMDs-based field effect transistors	P28
Vittoria	**Urso**	Investigation of Kinetic Functionals applied to metal nanoparticles	P29

Abstracts

Tuesday 4th

Effect of defects and adsorbents on the performance of optoelectronic devices based on atomically thin materials.

Paola Barbara
Department of Physics, Georgetown University, Washington, DC 20057, USA

Abstract:
Atomically thin materials have emerged as a promising platform for optoelectronics applications, due to their strong light absorption and their suitability for flexible substrates. Although a variety of high-performance optoelectronic devices have already been demonstrated, most of them were fabricated using monolayer, single-crystal flakes exfoliated from bulk material, therefore scalability is still a crucial issue. In the past few years, there has been significant progress in the synthesis of large-area, high-quality monolayer materials, but the effect of their low crystallinity and of the defects created by processing on the performance of devices is still unclear. Here I will discuss our recent work on different types of photodetectors based on large-area monolayers of a gapless material, graphene, and a semiconducting material, molybdenum disulfide [1-5]. We find that defects and adsorbates play an important role in the detection mechanism and that they can yield a substantial enhancement of the device responsivity.

References

[1] P. Han, E. Adler, Y. Liu, L. St. Marie, A. El Fatimy†, S. Melis, E. Van Keuren and P. Barbara, "Ambient Effects on Photogating in MoS_2", *Photodetectors*, submitted."
[2] A. El Fatimy, P. Han, N. Quirk, L. St. Marie, M. T. Dejarld, R. L. Myers-Ward, K. Daniels, S. Pavunny, D. K. Gaskill, Yigit Aytac, T. E. Murphy and P. Barbara, "Measurements of defect-induced cooling in graphene hot-electron bolometers", submitted.
[3] P. Han, L. St Marie, Q. X. Wang, N. Quirk, A. El Fatimy, M. Ishigami, P. Barbara, "Highly sensitive MoS_2 photodetectors with graphene contacts", *Nanotechnology 29*, 20 (2018).
[4] A. El Fatimy, A. Nath, B. D. Kong, A. K. Boyd, R. L. Myers-Ward, K. M. Daniels, M. M. Jadidi, T. E. Murphy, D. K. Gaskill, P. Barbara, "Ultra-broadband photodetectors based on epitaxial graphene quantum dots", *Nanophotonics 7 (4)*, 735-740 (2018).
[5] A. El Fatimy, R. L. Myers-Ward, A. K. Boyd, K. M. Daniels, D. K. Gaskill, P. Barbara, "Epitaxial graphene quantum dots for high-performance terahertz bolometers", *Nature Nanotechnology 11 (4)*, 335 (2016).

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Laser-irradiated 2D materials: a new path towards straintronic devices

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Abstract:
Graphene and transition metal dichalcogenides (TMDs) offer a unique platform to enable novel opto-electronic devices. Thanks to their peculiar physical and electronic properties such as bandgap tunability, chemical functionalisation and the ability to sustain high levels of strain, such materials can enable flexible photodetectors, highly-efficient solar cells and unforeseen "straintronic" devices, i.e. devices which electronic properties are tuned by strain. Laser-irradiation can be used to modify the properties of 2D materials to enable new devices. We demonstrate how laser-irradiation can be used to induce photo-oxidation in ultra-thin HfS_2. In this way, a spatially varying bandgap can be engineered using a local strain field to enable the first observation of the so-called "inverse charge-funnelling" [1], as illustrated in Figure 1. This effect allows photo-excited charges to be driven away from the excitation area, towards regions of smaller gap, where they can be efficiently separated and collected. We observe an enhanced signal, with a 350% improvement in the responsivity with respect to the pristine device, indicating efficient extraction of photogenerated carriers. The bias dependence of the photocurrent demonstrates that the measured signal is due to the inverse charge-funnelling enabled by the strain-engineered gradient of energy gap in the planar HfS_2/HfO_2 interface. Furthermore, photo-oxidation of HfS_2 leads to the formation of a high-k dielectric which can be easily embedded into a large number of devices comprising filed-effect transistors, resistive switching memories and optoelectronic devices [2]. Strain-engineering in 2D materials represents a new field with promising applications for a new generation of electronic devices, in particular when applied to graphene/hBN heterostructures [3].

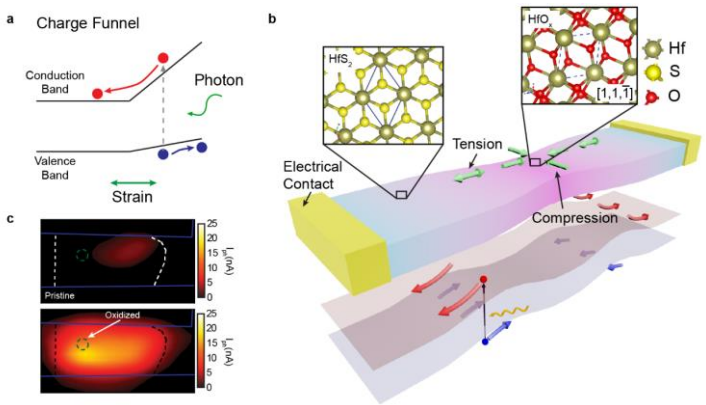

Figure 1. a) Charge-funnel concept. b) Selective oxidation lead to lattice mismatch at the interface between HfS_2 and HfO_x creating a strain gradiend which modulates the bandgap. c) Enhanced photoresponse is observed in proximity of the oxidised area.

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Electronic Detection of Oxygen Adsorption and Size-Specific Doping of Few-Atom Gold Clusters on Graphene

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Abstract:
Graphene's two-dimensional nature makes it very susceptible to adparticles: adsorbed atoms or molecules, either individual or clustered. For instance, graphene's electronic properties have been shown to be susceptible to gas molecule adsorption with a sensitivity down to single molecule detection [1]. Small clusters exhibit distinct electronic and structural properties that vary in a non-scalable way with their size. Theoretical investigations of few-atom metallic clusters as adparticles on graphene suggest that the cluster's size-dependent properties get carried over in, for instance, graphene's electronic properties [2].
We investigated the interaction between size-selected Au_2, Au_3, and Au_6 clusters and graphene. Hereto, preformed clusters are deposited on graphene field-effect transistors, an approach which offers a high control over the number of atoms per cluster, the deposition energy, and the deposited density [3]. A major part of the deposited clusters remains on the graphene flake as individual entities. In situ electronic transport measurements on cluster-graphene devices shows size-dependent charge transfer, and hence doping, which is detectable in field-effect measurements (see figure). We also investigated the binding of molecular oxygen to the cluster-graphene system. O_2 adsorbs with significant binding energy on the gold clusters [4]. The observed size-dependent effects are in agreement with charge transfers obtained from DFT simulations. This approach provides perspectives for electronic and chemical sensing of metallic clusters down to their atom-by-atom size-specific properties, and exploiting the tunability of clusters for tailoring properties in graphene.

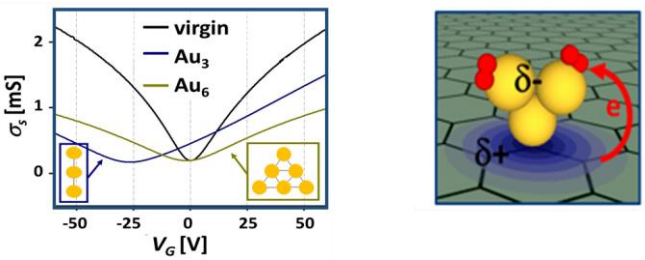

Figure: Left – sheet conductivity of the graphene device as function of the gate voltage, reflecting size-specific (n-type) doping of soft-landed Au_3 and Au_6. Right – schematic illustration of the charge transfers following oxygen adsorption on Au_3/graphene.

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Graphene quantum dots as smart nano-carriers for cancer therapy

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Abstract:
Graphene quantum dots (GQD), fragments limited in size of a single-layer two-dimensional graphene,due to their outstanding physical, chemical and biological properties, have shown promising applications in cancer therapy [1]. When compared with other carbon-based nanomaterials, GQD originating from graphene sources,exhibit particularlyunusual chemical/physical properties, such as low toxicity, chemical inertness, water solubility, and biocompatibility, which make them ideal nano-carriers for drug delivery; these nanomaterials alsoproved to improve the chemotherapy efficacy of anticancer agents acting at the nuclear level [2]. Moreover, the quantumconfinement, which confers fluorescence to these nanostructures, allows the simultaneous detectionand treatment of cancer cells, making them suitable platforms for theranostic purposes [3]. The presence of different reactive groups on the graphene surface allows theirmultimodal covalent and non-covalent conjugation with drugs, targeting ligands, and polymers, inorder to improve their pharmacological profile both *in vitro* than *in vivo* [4, 5]. GQD, synthesized by acidic oxidation and exfoliation of multi-walled carbon nanotubes (MWCNT) have been conjugated with anticancer agents and with targeting ligands that could specifically recognize specific receptors on the cells surface and induce receptor-mediated endocytosis in order to minimize the systemic toxicity and undesirable side effects typically associated with conventional therapy (Fig. 1).The reported results lead to targeted therapies forcancer treatment, opening new possibilities in the use of anticancer drugs poorly soluble in water andendowed with systemic toxicity.

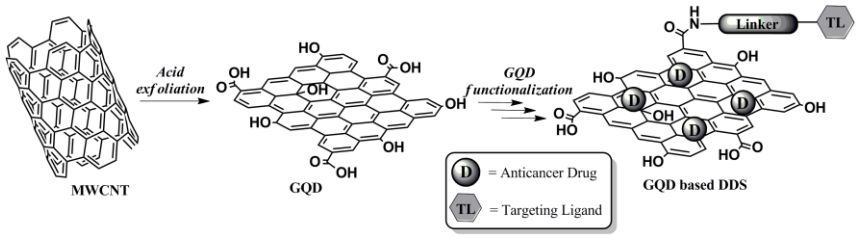

Fig. 1: Drug Delivery Systems GQD based for anticancer therapy.

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Molecularly imprinted nanogels combined to plastic optical fibre: influence of the nanostructure to the sensor response

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Abstract:
Polymer biomimetics prepared by the technique of molecular imprinting (MIPs), i.e. a template assisted synthesis [1], are synthetic alternatives to natural receptors that possess recognition properties similar to their natural counterparts (antibodies, receptors), but share the robustness and integrability to sensing devices typical of the polymeric materials.
MIPs can be prepared towards a wide spectrum of analytes, ranging from small molecules to proteins [2] and can be shaped in formats from micron- to nano-dimensions. Over the last few years the downsizing of the MIPs to nanoMIPs has shown to bring significant advantages in terms of binding kinetics, accessibility of the binding sites, homogeneity of the imprints, quasi-protein-sized dimensions, strengthening further their resemblance to natural receptors. Thus nanoMIPs appears as "plastic antibodies" [3] and are foreseen as ideal to be integrated to sensors [4].
Here we report on the optical effects that can be obtained by the integration of MIP nanostructures characterized by solvent-responsive properties to SPR sensing on a D-shaped plastic optical fibre (POF) [5], this latter chosen for the versatility of configurations offered, the easy and low cost of manipulation, the great numerical aperture, the large diameter, the possibility to withstand smaller bend radii than glass, the use of white light sources and the remote interrogation.
Experimental evidences showed that the solvent-responsible nanoMIPs when combined to the POF enabled to modulate the optical response just by exploiting the solvent-induced conformational rearrangements of the nanoMIP, that occurs right at the proximity of the plasmonic surface. These responsive nanoMIPs permitted to actively modulate the resonance wavelength shifts, hence the optical signal, alike a polymer switch. When used for sensing a model protein analyte, the nanoMIP-POF showed to reach ultralow detection limits.

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Electrospun nanocomposite nanofibers in chemical sensors for gaseous compounds

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Abstract:

Environmental monitoring is a world growing need owing to the strong impact of several anthropogenic activities on both human and planet health.

Air quality monitoring is generally performed with specialized equipment and analytical methods by regulatory agencies and researchers.

However, in order to obtain more realistic and continuous results on the situation of pollutants distribution, EU projects guidelines report the need to involve also citizens in environmental monitoring, thus low-cost and easy-to-use technologies are required.

To achieve this aim, innovative sensors for environmental monitoring have been designed and fabricated to date to obtain reliable values comparable to those provided by standard methods and technologies.

Among the main drivers for the design of advanced chemical sensors, the key characteristics include sensitivity, selectivity, and rapid responses. Over the last decade, the combination of nanostructured materials with many transducers has boosted the advances in this area, leading to significant enhancements in their sensing performance. These joint materials benefit from the synergy between doping agents (metal nanoparticles/rods/stars, metal oxide-nanoparticles/rods, quantum dots/rods, organic macromolecules, etc.) and the hosting nanostructures (i.e. polymer, metal-oxide, etc.): they are both on similar length scales and with a very large interfacial surface area when compared to the volume of the resulting material.

Currently, electrospinning is considered as one of the most versatile and inexpensive manufacturing technologies to design and develop nanostructured sensors to detect gases and volatile organic compounds (VOCs) in the air.

Sensors based on polymeric as well as metal-oxide fibers look extremely attractive for the low cost and great versatility of the raw materials that can be easily tunable, according to the transducer used and the application of interest, taking part to the resulting sensing features (selectivity and sensitivity).

The inclusion of variously working nanoparticles with different strategies of functionalization has allowed the sensors to achieve excellent performances under various points of view, ranging from robustness, to life-time, to sensitivity and selectivity.

Some experiences will be here described.

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Ion imprinting with graphene oxide and its application in electrochemical sensing

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Abstract:
Since about a decade ago, great number of works have been published on employment of graphene oxide (GO) nanoparticles in electrochemical sensing. GO is favored because of its solubility, nanoparticle shape (single-atom layers with large surface area) and surface properties where especially surface carboxyls are of great importance because they make GO great absorbent of heavy metals (HM) – an important environmental pollutants. In this work divalent HM cations were employed to self-assemble GO sheets in such a way that they formed the GO/HM complex. Consequently, after HM leaching, an "ion imprinted" nanostructure was left, i.e. a structure containing pores and sites accurate for a specific HM bonding. Thus a selectivity is gained for a HM electrochemical sensor prepared from the GO-based ion imprinted nanostructure. Furthermore, this nanostructure is easy to prepare, without a need of cumbersome synthesis of specially designed ion imprinted polymers. The part of the work was also an assessment of an electrochemical HM detection in real environmental samples employing electrodes modified with the prepared GO-based ion imprinted nanostructure.

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Structural Changes on Supramolecular Organization of Bitumen Induced by Advanced MWCNTs Based on Silica: Physical Chemistry Characterization

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Abstract:
In the 1991, Ijima discovered that it was possible to form carbon nanotubes (CNTs) under conditions similar to those used for the preparation of fullerene. A CNTs is a one-atom thick sheet of graphite rolled up into a seamless hollow cylinder with a diameter of the order of one nanometer. In this study the use of a new advanced MWCNTs based on silica support was tested, investigating their ability to modify the supramolecular organization of colloidal bitumen by shear dynamic rheological analysis. The MWCNTs under investigation were laboratory-synthesized products by CCVD (Catalytic Chemical Vapor Deposition), supplied by a University start-up named InnovaCarbon. Several physical chemistry techniques were used to characterize MWCNTs in order to understand the mechanisms that govern the interaction CNTs-asphaltenes micelles. The modification of the binder with the MWCNTs on silica based support increases the bitumen transition temperature from viscoelastic to liquid system, showing an excellent elastic resistance. In general, the CNTs give higher elastic modulus and tensile strength than the most common additives for building materials. In particular, the tested silica based nanotubes enhance strongly the viscoelastic characteristics. This investigation fits the recent research on bituminous binders with aiming to find new additives that can increase the performance and the lifetime of the asphalt. In order to evaluate the improvement made by MWCNTs-Silica, the effects of common commercial products were evaluated too. Overall, the results showed that a minimum amount of MWCNTs Silica (1wt. %) could shift the transition temperature of around 20°C. The time-cure test for the bitumen modified with MWCNTs Silica showed a flattened curve for the loss tangent throughout a wide range of temperature before to diverge toward its limiting value t*. That peculiar mechanical response may be due to a sort of viscoelastic buffering effect induced above the threshold amount of CNTs dispersed into bitumen. Within literature, similar rheological behaviors were observed for SBS modified bitumens. Finally, the authors hope that the presented approach can promote a new research method based on the chemical-physical characterization of nanomaterials usable for road paving.

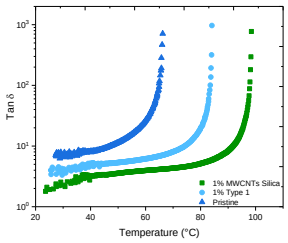

Figure 1. Semi-log plot of temperature ramp test for the pristine and modified bitume.

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Advanced field effect control of semiconductor nanowire-based devices

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Abstract:
The electrostatic control of semiconductor nanodevices by exploiting the field effect is ubiquitous in nanoscience and technology and traditionally follows the metal-oxide-semiconductor approach [1,2].
In parallel to the MOSFET approach, we explored different routes for achieving higher degree of field-effect manipulation in nanoscale semiconductor devices. One routes envisions the use of metallic finger gates to exploit the quantum confined Stark effect. This allowed us to achieve full control of individual charge and spin degrees of freedom in nanowire quantum dot systems [3] and to investigate the tunneling rates [4].
A second route, with a true paradigm change, envisions the use of soft-matter as the gate medium for applying impressively high static electric fields to semiconductors. This route exploits the way of *iontronics* to electrostatic gating, using the movement and arrangement of ions to build up an electric double layer that is the ultimate responsible for the electrostatic gating. Applied first to 2D materials, this approach is rising great promise also for application with other types of semiconductor nanostructures such as nanowires. Recently we proposed the use of ionic liquids as gate media for III-V semiconductor nanowire-based devices, demonstrating unprecedented gating efficiency and gate-induced change of the temperature behavior in the device [5]. We investigate the ionic liquid dynamics with atomistic simulations, correlating the hysteretic features to the microscopic parameters of the ionic liquid. Based on these results, we develop innovative device architectures exploiting the electric double layer gating for thermal management and energy harvesting at the nanoscale [6].

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Towards ultrafast and highly efficient optoelectronic devices based on III–V nanowires

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Abstract:

III–V semiconductor nanowires show great promise as nanocomponents of future high-performance optoelectronic devices, with applications ranging from solar energy harvesting to terahertz communications systems. These nanowires can be fabricated in a scalable, reproducible and tightly controlled manner by metalorganic chemical vapour deposition (MOCVD). Two methods are commonly used for the MOCVD of nanowires: (i) the vapour–liquid–solid (VLS) method using Au nanoparticles to drive anisotropic growth and (ii) selective area epitaxy (SAE) in which nanowires nucleate selectively in unmasked areas on the substrate. The VLS method has the advantages of tight control over the crystal structure (zinc-blende or wurtzite) and straightforward fabrication of radial (core–shell) heterostructures. SAE is more suitable for the fabrication of axial heterostructures and axially-doped homostructures, and is more compatible with Si substrates, enabling the monolithic integration of III–V nanowires with conventional Si microelectronics. The choice of growth method therefore depends on the ultimate device structure and the intended application. VLS-grown zinc-blende GaAs nanowires exhibit very short charge carrier lifetimes of under 5 ps, and high electron mobilities above 1000 $cm^2V^{-1}s^{-1}$ [1]. These properties make them useful for ultrafast optoelectronics. For example, films of aligned GaAs nanowires have been employed as THz polarizers that can be modulated on picosecond timescales [2]. SAE-grown InP nanowires, which exhibit long charge carrier lifetimes of over 1 ns, are currently being developed as the light absorbing and carrier transport materials in highly efficient solar cells.

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Chemical sensing with ZnO nano and microwires

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Abstract:
ZnO is one of the most important semiconducting materials in developing high-quality optical microcavities and high-efficiency ultraviolet (UV) optoelectronic devices owing to its direct wide band gap (3.37 eV) and large exciton binding energy (60 meV) [1]. Beside this, it is well known as chemical sensor since its surface interact with gases and a modification of electrical or optical properties is recorded [2]. ZnO crystallize in wurtzite structure and can be easily obtained as nanowire (NW) by different techniques (chemical or physical deposition), ensuring high surface to volume ratio available for interaction with gases. ZnO nanorods obtained by RF sputtering were investigated as conductometric gas sensors as a whole demonstrating excellent properties for H2S and H2 detection.
To better understand the properties of the ZnO NWs we investigated a single NW, instead of mesh of NWs with a wide diameters distribution. The individual nano/micro wire was studied by micro-PL spectroscopy in air and in controlled gaseous environment. PL imaging of the individual nano/microwire was studied in different atmospheric conditions for ZnO nanorods. When the diameter of the nanowire is high enough (up to microwire), Whispering Gallery
Modes (WGM) can be observed. We observed WGM and Fabry Perot modes in micron-sized wires of ZnO, that behave as high-quality active optical microcavities. We studied the conditions needed to exploit WGM for gas sensing applications.

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Hybrid Nanowire Based Quantum Networks at Atomic Scale: from growth mechanisms to properties

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Abstract:
Nanotechnology allows modifying the structure of nanoobjects down to the atomic scale. Low dimensional quantum heterostructures can be created in a nanowire system in order to modify its properties at will, e.g.: hybrid semiconductor-superconductor nanowire based quantum networks.
The aim of these new hybrid systems is to take advantage of Majorana pairs as the building blocks for the generation of qubits, which are the fundamental units of information in quantum computation. The configuration that would suit this application the most is the interface between a semiconductor and a superconductor, and an appropriate way to build them is to arrange them in a nanowire, which creates the so-called concept of proximitized nanowires. The selected semiconductors are usually InAs or InSb, while Al is mainly used as the superconductor, due to its theoretical transition to topological phase under certain chemical potential and external applied magnetic field conditions. In fact, reaching the material's topological phase is a fundamental requirement to achieve the Majorana Zero Modes (MZMs). Indeed, in order to achieve in the future a direct observation of the theoretical properties of the MZMs, defect free, relaxed and perfectly epitaxial heterostructures are needed. These newly developed hybrid quantum devices benefit from the new advances in growth methodologies. However, in order to obtain the most outstanding conditions to achieve the MZMs we will need to assure perfect growth conditions. In the present work, we will present how an accurate knowledge on the atomic positions, down to single atom detection, may help to deeply understand the improved properties of our complex nanowire heterostructures. We will show how from scanning transmission electron microscopy (STEM) and related spectroscopies, it is possible to obtain precise 3D atomic models of our hybrid systems and understand the growth mechanisms in detail. Atomic scale strain studies will allow observing the different relaxation mechanisms based on plastic and elastic deformations and visualize the defects induced to the nanowire structures that might be detrimental of their quantum properties. Special attention will be put on the superconductor-semiconductor heterointerface.

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Bottom-up and Top-down Fabrication of GaN Nanowires in Molecular Beam Epitaxy

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Abstract:
The bottom-up fabrication of compound semiconductors in the form of nanowires lifts the most fundamental constraint in epitaxial growth, namely, the necessity of using a substrate with a compatible crystal structure as well as similar in-plane lattice constants and thermal expansion coefficients. The lack of such a constraint allows the combination of highly dissimilar materials, thus paving the way for both improved functionalities and novel applications. Nevertheless, the bottom-up fabrication of semiconducting nanowires also suffer from certain disadvantages with respect to the synthesis of epitaxial films. Specifically, the nonideal growth conditions often required to promote either uniaxial or radial growth may favor the incorporation of higher concentrations of impurities and defects. Furthermore, the different chemical and physical properties of the precursors, which are simultaneously deposited on different crystal facets, can result in the formation of nanowire heterostructures with detrimental compositional and structural inhomogenities. In contrast to bottom-up methods, top-down approaches do not allow the combination of dissimilar material systems but facilitate the formation of nanowire heterostructures with extremely well-defined chemical and structural properties. Therefore, for those material systems for which their epitaxial growth has reached a high level of maturity, top-down fabrication methods are an interesting alternative to exploit the potential advantages offered by the nanowire architecture to improve the performance and functionalities of semiconducting devices.

Here, I will present an overview on the formation of GaN nanowire arrays in molecular beam epitaxy using bottom-up and top-down methods. With respect to the bottom-up approach, I will review the physical mechanisms responsible for the spontaneous formation of single crystalline GaN nanowires on a wide variety of substrates, including crystalline semiconductors (e.g. Si, SiC), amorphous materials (e.g. SiO_2, Al_xO_y), and different metals in the form of films and flexible foils. Regarding top-down methods, I will discuss a novel approach, coined selective area sublimation, which enables the facile formation of random and ordered arrays of GaN nanowires with a high luminous efficiency. This process, which is not based on reactive ion etching but on material sublimation in vacuum, can be monitored in-situ by reflection high-energy electron diffraction and line-of-sight quadrupole mass spectrometry. Selective area sublimation is thus found to be an efficient and easily controllable top-down approach that could be readily extended to other types of micro- and nanostructures as well as to additional material systems with similar crystallographic properties such as ZnO.

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Synthesis, characterization and chemical functionalization of germanium nanowires

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Abstract:
Functionalised nanostructures are a viable approach to realise detectors with high sensitivity and very limited weight and electrical consumption, thanks to their high surface/volume ratio. Germanium nanowires (NWs) are proposed here as a fundamental building block of a sensor to detect traces of explosives molecules (in particular TNT), down to a detection limit of ~$1x10^{-6}$ ppt.
In this communication we will report on the growth, structural and electrical characterization of these nanostructures. The first experiments on chemical functionalization tailored to bind the aromatic ring of TNT to the nanostructure will be presented. Germanium NWs were grown by Vapor Phase Epitaxy using iso buthyl germanium as a novel Ge source, at temperatures ranging from 340 to 460°C on (001) and (111) silicon and germanium substrates. Gold nanoparticles of different size (20-80 nm) were used as catalyst. The optimization of the growth procedure resulted in Ge NWs to 20 □m in length.
Details of the growth process and the growth conditions will be discussed, with particular emphasis on the control of the length of the NWs and their tapering. Different NW density and orientations are obtained, depending on the precursor flow and on the substrate orientation. The NW crystalline structure was observed by Transmission Electron Microscopy (TEM), evidencing their high structural quality.
The NWs were detached from the substrates with ultrasonication and dispersed on a carrier substrate with Au interdigitated electrodes. Single NWs were observed with Scanning Electron Microscopy (SEM) and contacted to Au electrodes with Pt deposited by Focused Ion Beam (FIB). Pt contacts were deposited with 50 pA and 30 kV ion beam current and acceleration voltage, respectively, at each ends of the NW. Linear I-V characteristics showed the ohmic nature of Pt-NW contacts. From RT resistance measurements, using two-terminal configuration, we obtained NW electrical resistivity values in the 0.05 - 0.5 ohm cm range. We propose the functionalization of the NWs surface with long chain alkanethiols terminating with an amino group, in order to provide the explosives recognition elements. Besides providing passivation of the NWs surface, the electron-rich amino groups will bind the electron-deficient explosive molecules of TNT through charge-transfer donor-acceptor interactions, thus causing sharp changes in the conductance of the electrical-sensing nanoelements.

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Wednesday 5th

Growth and Applications of Hexagonal Boron Nitride

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Abstract:
Large-scale growth of high-quality hexagonal boron nitride (h-BN) has been a challenge in two-dimensional (2D)-material-based electronic and energy devices. In this talk, I will demonstrate wafer-scale and wrinkle-free epitaxial growth of multi-layer h-BN on a sapphire substrate by using high-temperature and low-pressure chemical vapor deposition. Microscopic and spectroscopic investigations and theoretical calculations reveal that synthesized h-BN has a single rotational orientation with Bernal stacking order. A facile method for transferring h-BN onto other target substrates were developed, which provides the opportunity for using h-BN as a substrate in practical electronic circuits. A graphene field effect transistor fabricated on our h-BN sheets shows highly improved carrier mobility, because the ultra-flatness of the h-BN surface can reduce the substrate-induced degradation of the carrier mobility of 2D materials. Afterwards, I will show some potential applications of h-BN for a shell layer capping Au nanoparticles in surface-enhance Raman scattering, an encapsulation (or passivation) layer to protect unstable transition metal dichalcogenides (TMDs), and a proton exchange membrane to replace the Nafion film in a polymer electrolyte membrane (PEM) fuel cell.

Recent Advances in the Growth of Transition Metal Dichalcogenides by Vapour-Phase Approaches

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Abstract:

One of the simplest routes to the synthesis of transition metal dichalcogenides (TMDs) is the reaction of thin films of transition metal with chalcogen precursors, sometimes referred to as thermally assisted conversion (TAC). This method is potentially scalable, affords control over layer thickness, and offers compatibility with standard semiconductor processing techniques[1].

In this presentation, recent advances in TAC growth of $PtSe_2$, and related materials, will be described in detail. $PtSe_2$ can be grown at relatively low temperature suggesting potential compatibility with back-end-of-line (BEOL) processing. This low growth temperature also enables growth on glass and other substrates which would not survive the temperatures associated with typical vapour-phase growth processes. While the material grown by the TAC approach is polycrystalline it has nonetheless shown promise for applications in diverse areas such as sensing[2, 3] and (opto)electronics [4, 5].

A modified TAC approach for the synthesis of transition metal ditellurides will also be outlined. This entails the electrodeposition of Te layers onto predeposited transition metal films with subsequent conversion to TMD layers[6]. This approach allows for the synthesis of scarcely-studied TMDs including $PtTe_2$, which is a promising candidate for applications in electrocatalysis.

Finally, recent results on the synthesis of high-quality TMDs by a chemical vapour deposition (CVD) process, using a simple microreactor, will be detailed. This approach results in films with much higher crystallinity than those grown by TAC – albeit with less control over surface coverage and layer thickness. The use of such methods to grow TMD heterostructures will be outlined.

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Structure and Dynamics of Alkali-Metal Intercalated Black Phosphorus

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Abstract:

Phosphorene, i.e. single or few-layer sheets of black phosphorus (BP), raised the interest of the scientific community due to its many unusual properties. In particular, intercalation with potassium leads to a tuneable direct band gap, which makes the material suited for (opto)electronics, or intercalation with sodium could be of use for energy storage. In this work, we investigated BP after intercalation with different alkali metals by *in-situ* X-ray diffraction. The structure was determined directly after synthesis [1, 2] and structural development was followed in specific longer time intervals to determine the stability of the respective compound. A careful analysis of the time evolution of the diffraction patterns enables following the dynamics of the intercalated systems, which are dependent not only on the type but also on the concentration of the respective alkali metal.

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Growth and application of $MoTe_2$, WTe_2 and $PtTe_2$ films

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Abstract:
The interest in transition metal ditellurides has grown hugely over the last number of years, having previously been much less explored than the equivalent sulfide and selenide TMDs. This has led to reports of a host of interesting properties and applications such as $MoTe_2$ for phase-change applications, WTe_2 as a possible interconnect material and WTe_2 showing giant magnetoresistance [1, 2].
This work demonstrates an efficient method to produce phase-pure 1T' $MoTe_2$ films at temperatures as low as 450˚C. This is achieved through reaction of pre-deposited Mo and electrodeposited Te layers in an inert atmosphere [3]. The growth mechanism is further extended to produce films of WTe_2 and the lesser studied $PtTe_2$.
The $MoTe_2$ films demonstrate promising electrocatalytic results for the hydrogen evolution reaction with competitive slopes below 70 mV dec^{-1}. The $PtTe_2$ films are investigated as a catalyst for oxygen reduction. While the morphology of the WTe_2 films result in interesting single-crystalline flakes which are isolated and examined electrically.

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Ge-based layered materials with high anisotropy

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Abstract:
The research interest towards two-dimensional (2D) layered materials has been rapidly growing since the isolation of graphene [1]. Two are probably the main reasons for this boom. Firstly, they exhibit exceptional properties [2], often superior to their bulk counterparts; secondly, they can be easily produced via simple mechanical exfoliation, a technique which requires the availability of neither expensive equipment nor highly specialized technical personnel.
Among the numerous materials in this family, we are intrigued by those based on germanium. Notably, we are currently investigating the 2D semiconductors germanium arsenide (GeAs) and germanium sulfide (GeS). Both exhibit anisotropic nature, with strong anisotropic optical and electrical properties [3-5], and both have been recently attracting attention as photodetectors [3, 6].
However, there are so far very few literature studies; and too limited information is today available regarding their transport and optical properties. Here we will show the results of our investigation after characterization with polarized Raman spectroscopy, atomic force microscopy, X-ray photoemission spectroscopy and variable-temperature electrical measurements. We will also talk about the chemical stability in air of these materials, and how their degradation can be prevented or, in other cases, can be exploited depending on the desired applications.

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Intrinsic properties of molybdenum disulfide prepared by different methods

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Abstract:
The early research on 2D materials was based on exfoliated sheets, which are characterized by high crystallinity, but also by small areas and low yields. Another process to produce 2D materials was therefore quickly developed: the direct growth of materials in 2D sheets with the goal of the large-scale production. Because not every desirable substrate is suitable for direct growth, techniques were developed to transfer 2D materials from one substrate to another or to stack different 2D materials to heterostructures. However, 2D materials are extremely sensitive to their environment because of their atomically thin structure. Therefore, it still poses a challenge to maintain physical properties of 2D materials when prepared under different conditions.

For the 2D material molybdenum disulfide (MoS_2), Raman spectroscopy is an ideal method to compare differently prepared systems. With MoS_2, Raman spectroscopy can be used to make reproducible and rapid quantifications of strain and doping, properties both of which are strongly influenced by the environment. By using photoluminescence spectra such quantifications can be corroborated. We will show that grown 2D MoS_2 differ with respect to exfoliated 2D MoS_2. However, grown and subsequently transferred MoS_2 shows a very similar characteristic compared to exfoliated MoS_2, i.e. the n-doping increases and the strain decreases due to the transfer. A similar trend is observed for MoS_2-graphene heterostructures, built up either by transfer or by direct growth.

This shows that the coupling to the substrate plays a crucial role for the physical properties of MoS_2. The inclusion of water reduces the interaction with the substrate, thus the MoS_2 is less strained. However, the charge transfer from water leads to n-doping with respect to 2D MoS_2 on substrates without water inclusion. Consequently, the interaction is more important than the production method for the intrinsic properties of MoS_2, i.e. MoS_2 from growth processes and from exfoliation differ less than commonly assumed.

In order to create a strong interaction between substrate and 2D material, the system has to be prepared accordingly by avoiding water films or other impurities. The high temperatures during growth automatically clean the substrate, as a one-step cleaning and growth process. For exfoliation of MoS_2, a strong interaction with the substrate can be achieved by suitable pre-cleaning procedures. The latter is demonstrated for MoS_2 on gold.

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Graphene-like silicene grown on inert graphite surface

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Abstract

The challenge of designing groundbreaking systems, to connect with Si-based technology, has inspired the study of novel two-dimensional (2D) nanomaterials. Experimentally, 2D layers were first obtained by depositing Si atoms on metal (M) surfaces [1]. However, due to the strong p-d mixing between Si and M atoms, it is still debated if pure 2D-Si has been actually observed [2]. To minimize interactions and/or alloy formation, we have used highly oriented pyrolytic graphite (HOPG) as substrate. Indeed, due to the sp^2 configured C atoms, this substrate approximates better than M ones the properties of a honeycomb structure and it provides a higher chemical inertness. Based on scanning tunneling microscopy (STM) and Raman spectroscopy, we have reported that when Si atoms are deposited on HOPG surface at room temperature, they arrange in three configurations: silicene nanosheets [3] three [4] dimensional clusters and Si 2D nanosheets intercalated below the first top layer of carbon atoms [5]. In particular, Raman spectra showed a new feature, located at 542.5 cm^{-1}, that has not been reported so far for sp^3 Si modes, suggesting that we are dealing with a genuine vibrational silicene sp^2 mode with a low buckling configuration. Theoretical calculations of the structure and energetic viability of the silicene nanosheets, of the strain distribution on the outermost graphene layer and its influence on the Raman resonances support the reported experimental observations.

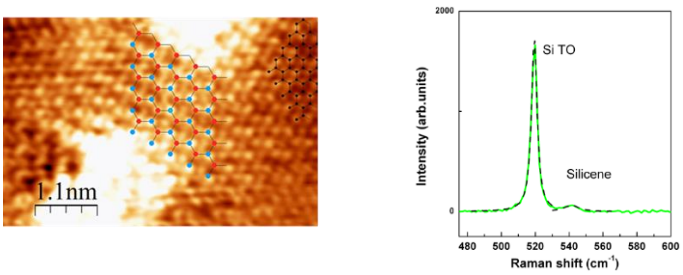

Fig. 1: Left: STM image (10.0 nm x 6.3 nm), obtained after Si 1ML deposition on HOPG at RT. A stick-and-ball model, representing Si atoms in a honeycomb and low buckled silicene arrangement, is superimposed as a guide for the eye. Note the presence of small, 1 nm high, silicon clusters (white regions). Right: Raman spectrum of the sample shown in the left panel.

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Growth and characterization of TMD heterostructures

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Abstract:

Two-dimensional (2D) materials, such as graphene and transition metal dichalcogenides (TMDs), are promising materials for numerous electronic applications. The properties of TMDs range from metallic to semiconducting suggesting the exciting prospect of creating devices solely from 2D materials through the use of heterostructures. The formation of heterostructures opens many opportunities such as improving the properties of the materials and band gap alignment.

In our research we used a single-step chemical vapor deposition (CVD) growth method in which a micro-reactor was used to synthesize $MoSe_2/WSe_2$ heterostructures.[1] This combination of ambipolar WSe_2 and n-type $MoSe_2$ allows the formation of an atomically-thin p-n junction without any further processing steps. This method allows the formation of both lateral and vertical heterostructures offering a range of device architecture possibilities. These structures were intensively studied by various characterization techniques such as (low-frequency) Raman spectroscopy, photoluminescence spectroscopy, x-ray photoelectron spectroscopy and atomic force microscopy (AFM) to obtain information on the structure, interfaces and properties of the heterostructures. Advanced AFM modes such as conductive AFM and Kelvin probe force microscopy offered further insight into these fascinating structures.

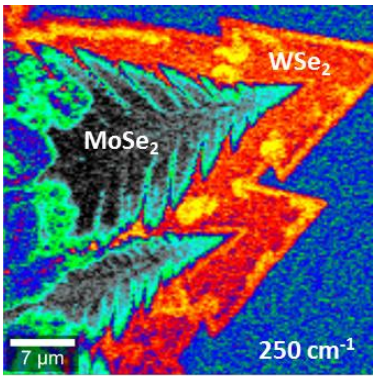

Figure 2: Raman intensity map at 250 cm^{-1} of a $MoSe_2/WSe_2$ heterostructure.

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Hierarchical carbon coated 3D-CZTS nano-structural anode material for high performance LIB applications

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Abstract:
Improving the energy density of the Li-ion battery (LIB) is the key challenge for its future applications. Therefore, development of novel electrode materials together with high areal capacity, faster electron transport kinetics, and improved Li-ion diffusion are currently the most active frontier's research areas for lithium-ion batteries. In this work, carbon coated hieratical 3D-CZTS nano-flowers (CZTS@C) has been fabricated utilizing hydrothermally synthesized CZTS nanoflower followed by facile carbon coating. The CZTS@C thus produced demonstrated enhanced electrical conductivity, improved Li-ion diffusivity and higher mechanical stress-strain tolerance over subsequent electrochemical cycling. The Li-ion battery electrode based on the optimized CZTS@C exhibits a high areal capacity around 1-2 mAh/cm^2 as well as high gravimetric capacity of 815-1210 mAh/g with good stability up to 100 cycles and high-rate capability of 1500, 920 and 425 mAh/g at current density of 500, 2000 and 5000 mA/g, respectively, which is superior to other metal chalcogenide materials. It's proposed that Li_2CO_3 formation as SEI layer in CZTS-C is an effective strategy for enhancing the areal capacity, columbic efficiency, and stability in LIB application of CZTS.

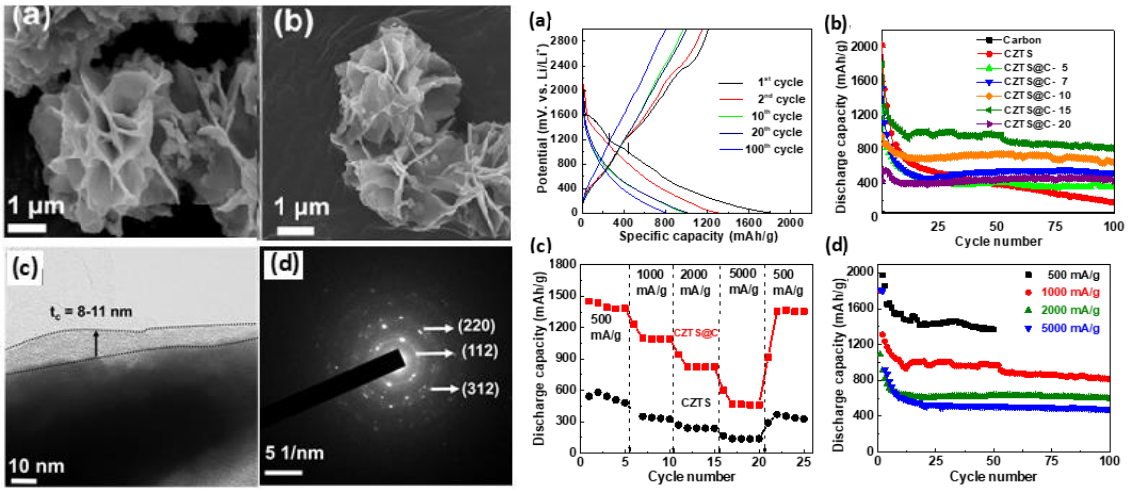

Figure (left) SEM and TEM images of the CZTS and C-CZTS samples; (right) Charge-discharge performance (a), Discharge capacity of different carbon contents up to 100 cycles (b), Capacity at different charging rates (c), and capacity at different charging rates (d) of the C-CZTS samples.

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From Liquid to Solid State: highly homogeneous, smooth, and transparent WS_2 – polymer films of of Liquid Exfoliated dispersion

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Abstract:
Since the graphene discovery and its presentation as the wonder material scientist around the globe started looking for similar and even better performing layered structures. As we know now there are thousands of layered crystals accessible although the materials show of their unique properties only when thinned down to few and monolayers often simultaneously opening their bandgap. The Liquid Phase Exfoliation is a method which enabled isolation of 2-dimensional (2D) nanomaterials with precise control of size, shape, composition and number of layers as well as monolayer content what is crucial for many applications.
In presented research tungsten disulphide (WS_2) dispersions with high population of single and few layers were prepared by LPE method. High quality of the 2D structures was verified with use of techniques like TEM, AFM UV-Vis, Raman Spectroscopy. Applying earlier developed size selection procedure, narrow lateral size distribution of WS_2 nanosheets in liquid dispersions was achieved. Further, monolayer enrichment procedure was demonstrated to successfully enrich liquid exfoliated WS_2 dispersions in monolayers, resulting with WS_2 monolayer contents of about 75%.
Although Liquid Exfoliated 2D materials exhibit a wide range of desirable for applications properties, such as narrow linewidth Photoluminescence, there is a significant drawback associated with them being dispersed in a liquid. For many applications such as transistors, it is required that the materials must be in a solid form. That is challenging without quenching the optical properties of the pristine form. Therefore, transfer from liquid to the solid state became undoubtedly important in nowadays research. The presented study will discuss preparation of highly homogenous, smooth and transparent WS_2 films in the polymer matrix, which will surely open doors for future electronics devices fabrication.

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Bio-applications of semiconductor nanowires

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Abstract

Semiconductor nanowires are very promising tools for biological applications. Their small dimensions, which are on the same length scale as many cell components, make them an ideal tool to probe and stimulate cells with minimal perturbation. In this talk I will review our work towards using nanowires for neural implant [1, 2] and biosensor applications [3-5], as well as our studies towards understanding and controlling the cell-nanowire interface [6, 7].

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New Pathways in the Synthesis of 2-Dimensional Materials

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Abstract:
Two-dimensional (2D) class of materials has attracted tremendous interest from both academia and industry due to their wealth of remarkable properties occurring as a result of their atomic thickness and infinite lateral dimensions. However, these 2D materials alone do not possess the properties that are required in a range of technological applications. Therefore, in order to enhance the conducting properties, it is important to blend it at the atomic level to get best performance. By simply decorating 2D materials with nanoparticles opens up other possibilities for new and unexpected phenomena. Our approach for making 2D based nanocomposites uses a clean, rapid technology. It potentially enables new advanced 2D inorganic nanocomposite functional materials designed and engineered in a unique manner by using superheated water with unusual properties. It utilises a green, rapid and Continuous Hydrothermal Flow Synthesis (CHFS) route for synthesis of 2D-inorganic nanocomposites. This affords advanced functional materials with minimal structural and electronic defect. The CHFS process involves mixing a flow of supercritical water with a flow of water-soluble precursor(s) (generally metal salt/s) to give rapid synthesis and controlled growth of nanomaterials in a continuous manner. Furthermore, the use of CHFS represents a highly tunable medium, where composites can be engineered *via* process parameters, e.g. with temperature and pressure. This single step synthetic approach not only enables control over oxidation state of materials (e.g. graphene), but also offers an optimal route for homogeneously producing and depositing highly crystalline nanostructures into 2D-materials. The process has many advantages; it does not utilise a complex and time-consuming process, limits the use of harmful chemicals, and effectively reduces the synthetic process time.

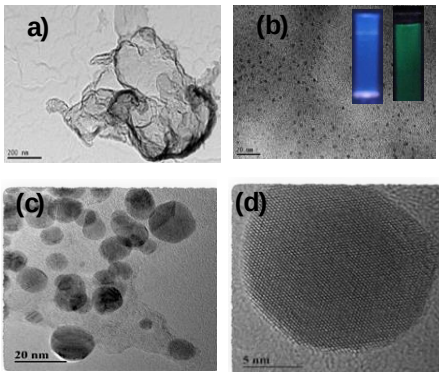

Figure. Trasmission Electron Microscopy images of a range of nanomaterials synthesised via CHFS (a) graphene sheet, (b) graphene quantum dots (inset) graphene quantum dot solution under UV light source (c) Ag-Graphene an

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Conduction Current and Displacement Current in Electric Generators

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Abstract:
Electric generators convert mechanical power into electric power and they provide most of electric power for industry and our daily life nowadays. Since the first electrostatic generator was invented more than 370 years ago, many types of electric generators have been reported till now. The working principles of converting mechanical power into electric power in these generators can be classified into three primary categories, i.e, electromagnetic induction, electrostatic induction and piezoelectric effect. Electromagnetic generators produce conduction current based on Faraday's law. In contrast, electrostatic generators and piezoelectric generators create displacement current under electrostatic induction and piezoelectric effect, respectively. In this talk, we present a new type of electric generators which could generate conduction current. These generators can be simply constructed using a pair of semiconducting or/and metallic electrodes which possess distinct chemical potentials. The generators can work in one of two working modes, i.e. the contact-separation mode and the sliding mode. In the contact-separation mode, electrons could diffuse from the high into the low chemical potential electrode once the two electrodes are brought in contact. A p-n junction, as well as a depletion region, is formed across the contacted surfaces. When the two electrodes are being separated, the diffused electrons are then discharged to the external circuit and flow back to the high chemical potential electrode, converting the mechanical power to electrical power. With a small load resistance, conduction current and displacement current are clearly seen in the contact-separation cycles. By contrast, one electrode can be slid on the other electrode in the sliding mode. Electrons are generated through triboelectrification process at the contacted surfaces and they are then quickly swept out of the p-n junction by the built-in electric field, forming a conduction current across the contacted surfaces.

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Perovskite solar cells

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Abstract:
Halide perovskites are quickly overrunning research activities in new materials for cost- effective and high-efficiency photovoltaic technologies. Since the first demonstration from Kojima and co-workers in 2009, several perovskite-based solar cells have been reported and certified with rapidly improving power conversion efficiency. Recent reports demonstrate that perovskites can compete with the most efficient inorganic materials, such as silicon and cadmium telluride, while they still allow processing from solution as a potential advantage to deliver a new cost-effective solar technology.
Compare to the impressive progress in power conversion efficiency, stability studies are rather poor and often controversial. An intrinsic complication comes from the fact that the stability of perovskite solar cells is strongly affected by any small difference in the device architecture, preparation procedure, materials composition and testing procedure.
In the present talk, we will focus on the stability of perovskite solar cells in working condition. We will discuss a measuring protocol to extract reliable and reproducible ageing data. We will present new materials and preparation procedures, which improve the device lifetime without giving up on high power conversion efficiency.

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Nanostructured Functional Polymers for Electrical Energy Storage

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Abstract:

We synthesized five new bottlebrush polymers using free radical polymerization as well as ring-opening metathesis polymerization (ROMP). These brush polymers contain different lengths of PEG side chains and two different backbones, polymethacrylate and polynorbornene. We like to present the influence of polymer architectures on mechanical stability, ionic conductivity, Li-ion transport number and electrochemical stability of a series of SPEs obtained thereof by mixing with different amounts of LiTFSI. We also compare the results to the respective linear PEG counterparts. The differences in battery parameters were analyzed and correlated with respect to thermal properties such as T_g and ΔH_{melt} in order to understand the fundamental factors which influence the properties of solvent-free PEG containing SPEs.

Additionally, we report the polymerization of glycidyl propargyl ether (GPE) by monomer-activated anionic ring-opening polymerization yielding clickable high molecular weight PEGs with very low dispersity. Fourier-transformation near-infrared spectroscopy was utilized for in-situ reaction monitoring and kinetic studies. Further, benzyl- and tri(ethylene glycol) pendant groups were quantitatively grafted to the P(GPE) backbone tuning the mechanical- and thermodynamic properties. As a consequence, this will strongly influence the electrochemical properties and opens the way for the use in battery systems. For the first time, sequential polymerization of GPE and glycidyl methyl ether (GME) to get block copolymers was shown to allow for a broad extension of this universal, clickable alkyne-functionalized PEG platform.

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VACNT growth on Aluminium: towards innovative supercapacitor nanocomposite electrodes

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Abstract:
The aim of this work is to develop innovative electrodes materials with high specific capacitance based on vertically aligned carbon nanotubes (VACNT) for supercapacitors. Catalytic chemical vapor deposition (CCVD) is one of the best method for VACNT growth. However considering the aluminium melting temperature (c.a. 660°C), the synthesis of VACNT on such substrates requires a significant reduction in the growth temperature as compared to conventional substrates [1-2]. Our approach was first to identify the most relevant synthesis parameters to achieve VACNT growth at such a low temperature by using precursor mixtures more favourable for a decomposition at low temperature [3]. Our results show that, with a single-step aerosol assisted CCVD process; it is possible to obtain clean, long and dense VACNTs on Al current collectors, with a growth rate at the best level of the state of the art at such low temperature. VACNT are then used to develop new pseudocapacitive electrode materials based on VACNT modified with Electronic Conducting Polymers (ECP) and/or metal oxide electrodeposited in a controlled manner [4]. Nanocomposite electrodes of poly-3-methylthiophene (P3MT) in ionic liquid and manganese oxide in aqueous electrolytes both homogeneously deposited on VACNT have been elaborated and their storage properties determined. Finally, we select best nanocomposite configurations for electrodes upscaling demonstrating the industrial feasibility of the approach.

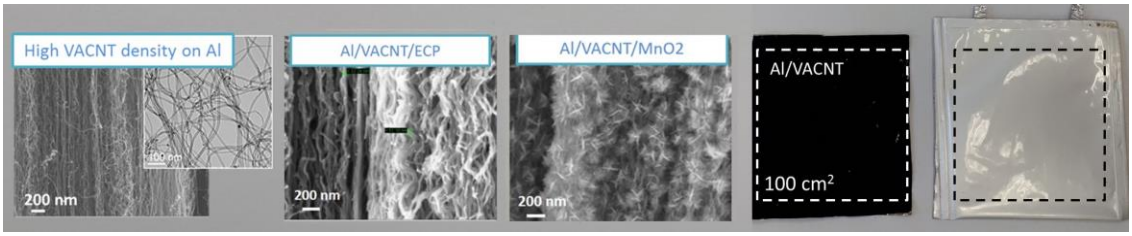

Figure: VACNT grown on Al current collectors, VACNT modified with PCE and metal oxide, upscaled VACNT/Al electrode and a pouch cell

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Composite nanostructures for energy harvesting

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Abstract:

Composite nanostructures can be efficiently applied for Sunlight detection and conversion and, more in general, for energy harvesting. In most of the applied systems, like photodetectors, excitonic solar cells and (photo)-electrochemical cells to produce solar fuels, nanomaterials can play a critical role in boosting photoconversion efficiency by ameliorating the processes of charge photogeneration, exciton dissociation and charge transport. Several strategies can be pursued, including broadening of light absorbance to reduce solar light losses, fastening exciton dissociation and charge injection from the photoactive medium to the charge transporting materials, reducing charge recombination during charge transport and collection at the electrodes. In this lecture, a few examples of application of nanocomposites will be thoroughly discussed, [1-5] highlighting the role of interface engineering to improve the efficiency of energy conversion from Sunlight to electric power and/or chemical fuels.

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Nanostructured materials for energy conversion

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Abstract:

The widespread adoption of clean energy converters such as proton exchange membrane fuel cells (PEMFC) is mainly hindered by the degradation of their component materials over time. To overcome this issue, original methods of elaboration are needed. Our approach is based on the use of nanofibres prepared by electrospinning and their multiscale assembly to produce PEMFC materials with specific architectures and improved properties. The size and morphology of the fibres and the macroporous architecture of the corresponding webs are expected to bring associated advanced properties, in particular with regard to mass transport and mechanical properties, with beneficial effects on the performance and lifetime of the resulting membrane-electrode assemblies.

Due to its inherent adaptability and versatility, electrospinning can be applied to all stages of the preparation of PEMFC materials, from electrolyte membranes to electrodes [1].

We are thus developing composite membranes based on ionomers embedding electrospun polymer webs, which demonstrated high mechanical resistance and durability while keeping high proton conductivity [2]. Current work aims at going beyond the simple role of mechanical reinforcement of nanofibrous webs by controlling the heterogeneity in the composite membranes *via* the interactions between nanofibers and ionomer matrix.

Our work also entails the preparation of nanofibrous electrocatalyst supports based on carbon, transition metals, metal carbides and oxides, with high durability and corrosion resistance [3]. The challenge to address is the use of highly porous self-standing webs as electrodes directly in the membrane-electrode assembly.

In parallel, Pt deposition techniques are investigated leading to extended metal surfaces onto the electrospun supports, such as Ni galvanostatic displacement, self-terminated Pt electrodeposition and electrochemical atomic layer deposition [4]. The thin film morphology will enable higher platinum exploitation and increased stability, leading to highly performing electrodes with ultra-low loading of the noble metal.

The assembly of these nanostructured materials will allow the development of a new generation of PEMFC cores, in which the components are fabricated by electrospinning and with the possibility of scale-up at industrial level.

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Annealing Temperature Grain Size dependence in Room Temperature Sputtered Gadolinium doped Ceria thin films for SOFC applications

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Abstract:
Solid Oxide Fuel Cells (SOFC) are electrochemical devices that can convert the chemical energy of a fuel in electrical and thermal energy with a great efficiency. Typical SOFC working temperatures are in the range 800°C ÷ 1000°C, using Yttrium stabilized Zirconia (YSZ) as electrolyte. This range of temperatures induces a fast degradation of the materials composing the cell itself and, consequently, a fast degradation of the chemical and electrical performances of the device. The use of a Gadolinium Doped Ceria (GDC) barrier layer between cathode electrode and YSZ electrolyte limits degrading materials' inter-diffusion processes. Furthermore, the presence of grain boundaries in the barrier layer increases the oxygen ion transport, improving the overall cell performance.
The present work illustrates SOFC performance improvement achieved through the deposition of a GDC thin film (400 nm) barrier layer using a Physical Vapor Deposition (PVD) technique, namely Room Temperature Sputtering, on screen printed half-cell (anode/electrolyte) provided by SOLIDpower S.p.A. After GDC addition, the cell has been completed with a screen-printed cathode. The obtained complete cell performance has been compared with that of a standard button cell manufactured by SOLIDpower S.p.A., by means of Electrochemical Impedance Spectroscopy (EIS) and j-V curve measurements. The comparison shows better performance of the cell with sputter deposited GDC in all the investigated cases. However, the performance changes with the post-growth annealing treatment. The choice of a suitable post-growth annealing process in terms of ramp and plateau temperature is therefore crucial to obtain the best cell performance, inducing a change in the grain size and in the number of grain boundaries present in the GDC layer.

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Electric transport and voltage-noise properties of granular aluminum oxide nanowires

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Abstract:

Granular aluminum oxide ($gAlO_x$) is a well-known material formed by a three-dimensional random network of nanosized aluminum particles, each covered by a rather uniform oxide layer. Its unusual superconducting properties have been recently investigated for application in quantum circuits. The intrinsic irregular structure of $gAlO_x$ requires, however, a good understanding of the transport properties and in particular of the effect of disorder, especially when patterned at the nanoscale level. In view of these aspects, electric transport and voltage fluctuation have been investigated on thin-film based AlO_x nanowires, in the normal state and at temperatures between 8 and 300 K. Nonlinear resistivity and two-level tunneling fluctuators have been observed. In order to identify the nature of the noise processes, different theoretical models have been considered and compared.

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Thursday 6th

Engineering thermal boundary conductance of a metal/polymer interface

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Abstract:
Printable, flexible organic electronics is based on polymers and other organic molecules, and have the advantages of reducing dependence on silicon and rare earth materials, in addition to being light and low cost. Heat management of organic electronics is a challenge due to the large density of interfaces between highly dissimilar materials, such as metals and polymers. Heat conduction in low dimensional materials is currently one of the unsolved fundamental scientific issues, especially in the case of an interface with characteristic length scales ranging from a few atoms to tens of nanometers between dissimilar materials. Here we used spin-coating to fabricate 1-15 nm thick polymer (polymethyl methacrylate, PMMA) films on silicon substrate and coated with ultra-thin gold film or gold film with a 2 nm titanium layer interfacing the polymer. We employed frequency-domain thermoreflectance (FDTR) to measure the effective thermal conductivity of the polymer films and hence obtained the thermal boundary conductance between metal and polymer. The PMMA thickness dependent thermal boundary conductance was revealed. The presence of titanium layer increased thermal boundary conductance to twofold, and attributed to the strengthened mechanical adhesion between titanium and polymer compared to the gold-polymer interface. These results help inform the engineering of metal/polymer interfaces for maximizing heat transfer.

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Transition metal dichalcogenides in back-gate field effect transistors

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Abstract:
Few-layer transition-metal dichalcogenides, such as MoS_2, WSe_2, or $PdSe_2$, have become very popular for electronic applications. Here, we discuss the current-voltage characteristics at high drain bias of bilayer MoS_2 transistors with Schottky contacts [1]. We show that oxidized Ti contacts form rectifying junctions on MoS_2 and cause asymmetric output characteristics, which we explain in terms of two back-to-back Schottky junctions with unbalanced barrier heights. We use MoS_2 transistors with ohmic contacts, at low drain bias, to investigate the photoconductive and photogating effects caused by charge trapping in extrinsic and intrinsic defects [2]. By focusing on the hysteretic transfer characteristics, we demonstrate that positive charge trapping is dominant in transistors with 2D-material channel and SiO_2 gate dielectric [3]. We investigate the effect of electron irradiation during the usual SEM imaging and show that its detrimental effect is partially recovered after a long time annealing at room temperature [4]. Finally, taking advantage from the n-type conduction, combined with the low workfunction, the sharp edge geometry, the lattice defects and the elasticity of the material, we demonstrate field emission current from few-layer MoS_2 and WSe_2, which is promising for vacuum electronic applications [4-6]. In particular, we prove that the field emission current can be modulated by a back gate and propose a new field emission transistor [6].

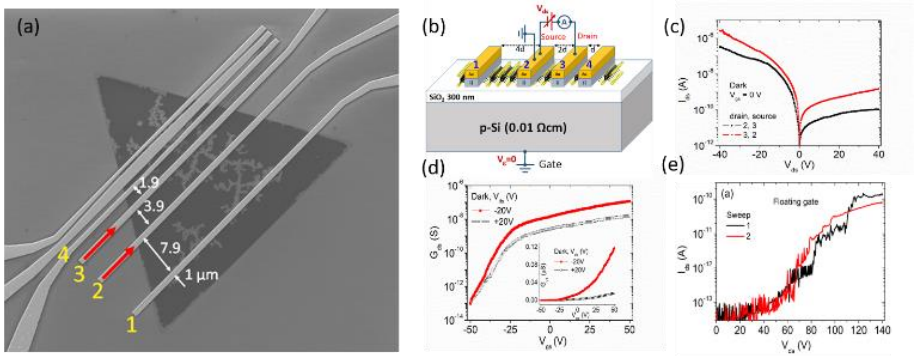

Figure 1: MoS_2 back-gate field effect transistor. (a) SEM top-view of a bilayer MoS_2 flake. (b) Layout of the transistor, (c) output and (d) transfer characteristics and (e) field emission current.

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Innovative Nano-Materials and Nanoscale Devices for the end of the Roadmap

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Abstract
We are facing many challenges for the end of the Nanoelectronic Roadmap in the next two decades dealing with power consumption, computing performance, variability and reliability. With respect to the needed substantial reduction of the static and dynamic power consumption of future high performance and/or ultra low power terascale integration of logic and autonomous nanosystems, new nanomaterials and novel nanodevice architectures are mandatory.

This paper presents some of the most promising solutions using ultimate Multigate NanoCMOS and Nanowire FETs, Small Slope Switches like Tunnel FETs and FeFET, and Hybrid Nanoscale Transistors such as Fe TFET, Phase Change Tunnel FET and Metal Filament MOSFET. To boost their electrical properties, these innovative nanodevices will be combined with advanced nanomaterials, including ultra-thin Si-Ge-III-V/OI, 2D layers (phosphorene, transition-metal dichalcogenides, etc.), 1D semimetals, and Heterostructures using strained Si, Ge and III-V materials.

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Scanning probe microscopy based fabrication and characterization of sub-micron Schottky junctions on as-grown graphene/Ge(100)

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Abstract:
Graphene is an extraordinary material showing outstanding physical properties suitable for a wide range of applications in electronics and optoelectronics. The CVD growth of graphene on germanium substrate acting as catalyst is an emerging method suitable for the development of CMOS compatible devices, given the absence of metal contamination typically present in metal-catalyzed (e.g. Cu) growth. In this work, we report on the fabrication of sub-micron sized graphene/Ge(100) Schottky junctions directly on as-grown graphene/Ge samples and their characterization using an approach fully based on scanning probe microscopy (SPM). SPM-lithography in the local anodic oxidation configuration was used for patterning. Protruding features (Fig. 1a)) up to several nanometers in thickness are produced by controlling tip translation rate and applied voltage. Conductive-AFM (c-AFM) measurements showed a highly non-conductive character of the patterned features. The capability of such lithographic approach to define graphene patches electrically isolated between each other was assessed by patterning a grid of perpendicular lines, followed by c-AFM measurements using the Ge substrate as collector electrode. Two-dimensional DC-current maps (Fig. 1b) show clearly the presence of graphene regions in which the current is almost uniform, which are surrounded by non-conductive lines (SPM-lithographic pattern). Moreover, DC I-V curves were collected by c-AFM on the graphene regions. The I-V characteristics showed a typical Schottky junction behavior and were analyzed to extract the main device parameters (barrier height, ideality factor, series resistance).

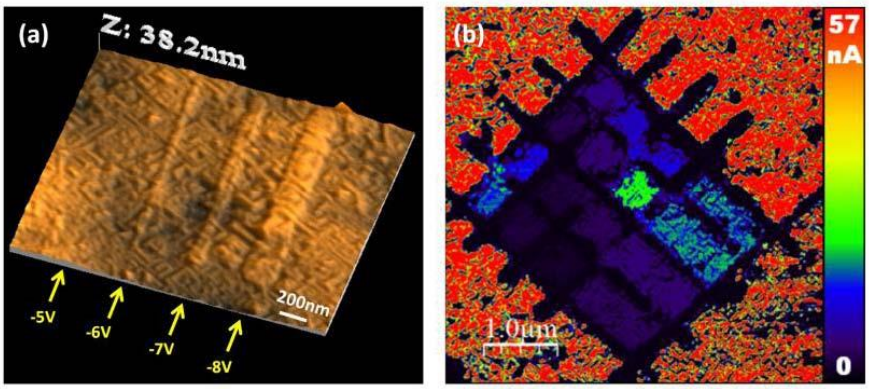

Fig1: a) 2D AFM map showing lithographic lines obtained at different applied voltage; the pattern is protruding from the typical ordered nanostructured surface shown by monolayer graphene/Ge(100); b) c-AFM map of graphene areas surrounded by SPM lithographic patterns.

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Electron-transporting perylene diimide films deposited by supersonic molecular beams

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Abstract:
In the last 15 years, perylene diimide derivatives functionalized in the bay region by the addition of cyano groups (C≡N) have attracted the attention of the scientific community as effective air-stable electron-transporting compounds [1]. N,N'-1H,1H-perfluorobutyl-1,6- dicyanoperylene-3,4:9,10-bis (dicarboximide) (PDIF-CN_2), in particular, has emerged as the reference material for analyzing the fundamental properties of n-type molecular semiconductors both in form of crystals and films.
In this contribution, we report on the growth of PDIF-CN_2 films, by the Supersonic Molecular Beam Deposition (SuMBD) technique, on SiO_2 dielectric surfaces for the fabrication of n-type transistors. In a SuMBD system, molecules are seeded in a hyperthermal carrier gas flow and their kinetic energies (Ek) can be enhanced by more than one order of magnitude, if compared with the conventional evaporation processes. In this study, PDIF- CN_2 films were grown by keeping the substrate at room temperature, while Ek was increased up to 17 eV and the deposition rate (R) was finely tuned from 0.01 and 0.22 nm/min. In these conditions, the PDIF-CN2 film growth mode displays a peculiar 3D character [2]. Just after the deposition, indeed, PDIF-CN2 films are not continuous being formed by separated hemispherical mounds (diameter D∼150 nm). Conversely, during the post-deposition period, a spontaneous wetting process of the condensate takes place ending up with the formation of continuous layers and the enhancement of the related electrical properties. This exotic phenomenon evolves with unusually long and R-dependent time scales. While for R around 0.1 nm/min, the PDIF-CN2 film reorganization is completed within 30 days and final charge mobility rises up to 0.2 $cm^2\ V^{-1}\ s^{-1}$, layers grown at R< 0.05 nm/min remain stably composed of isolated nano-domains. The film morphological evolution, described in terms Height-Height Correlation Function, was compared with theoretical simulations based on stochastic partial differential equations [3]. To better reproduce the experimental data, we found that the introduction of a surface equalizer term, characterized by a relaxation time taking into account the presence of a local mechanism of molecular correlation, is needed.

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Microwave plasmon resonance in high-mobility hBN-encapsulated graphene

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Abstract:
It has been shown that graphene field effect transistors are restricted to a 100GHz bandwidth by intrinsic effects [1]. To overcome that limit and pave the way for THz imaging or high-resolution RADAR applications one can take advantage of the large ballistic length [2] to realize GHz plasma resonance (PR) devices. Graphene is a well-recognized 2D material for plasmonics as illustrated in recent THz and mid-infrared optics experiments [3]. These high-energy plasmons however, couple to the dielectric surface modes giving rise to hybrid plasmon-polariton excitations. Ultra-long wavelengths address the low energy end of the plasmon spectrum, in the GHz–THz electronic domain, where intrinsic graphene Dirac plasmons are essentially decoupled from their environment. However, experiments are elusive due to the damping by ohmic losses at low frequencies. New fabrication techniques, in particular the encapsulation of graphene in hexagonal boron nitride (hBN), lead to extremely long electron mean free paths. We demonstrate here a micrometer size quarter-wave PR-capacitors using high-mobility hBN-encapsulated graphene characterized through its admittance in a broad 70 GHz frequency range at cryogenic temperature in the near-ballistic regime. We report a 100 μm quarter-wave plasmon mode, at 38 GHz, with a quality factor Q≈2 at 30K and n =$2\text{x}10^{12}$ cm^{-2} [4]. The doping and temperature dependencies is consistent with a velocity $v_{pl}\approx 4.v_F$ characteristic of screened plasmons. Fitting the complex admittance spectra with a distributive transmission line model yields a precise determination of the electronic properties of our graphene device (electronic compressibility, kinetic inductance, and mean free-path) and plasmon characteristics (velocity and impedance), in good agreement with theory. This GHz frequency capacitor experiment constitutes a first step towards the demonstration of ballistic plasma resonance transistors for microwave detection in the sub-THz domain and room temperature for wireless communication and sensing. It also paves the way for the realization of doping-modulated superlattices where plasmon propagation is controlled by Klein tunneling.

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Investigating the Electronic Properties of Oxide/MoS_2 Interfaces

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Abstract:
One of the principal factors motivating the study of 2 dimensional semiconductors in insulating gate electron devices is the potential for 2D semiconductor systems to result in near ideal semiconductor/oxide interface properties, with associated performance enhancements for MOSFET and tunnel FET devices. This presentation will focus on the application of impedance spectroscopy (100Hz to 1 MHz) to the analysis of interface states and border traps in the oxide/MoS_2 system using MOS and MOSFET structures. The experimental capacitance-voltage (CV) and conductance-voltage (GV) response over frequency and applied bias are analyzed in conjunction with physics based *ac* simulations to probe the density and energy distribution of oxide/MoS_2 interface states and border traps in the oxide.

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Mesoscopic Percolating Resistance Network in Reduced Graphene Oxide Thin Film

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Abstract:
Solution processing is emerging as one of the most attractive way to produce and to process large quantities of graphene and related materials (GRMs) at highly competitive costs for a wide range of application based on printed electronics [1]. In view of their highest surface-to-volume ratio, GRMs are also particularly appealing as nanofillers for polymer composites [2]. GRMs are intrinsically disordered on multiple length scales incorporating local geometrical defects, holes, as well as a large amount of chemical functionalization. Several efforts have been devoted in last years to study the charge transport at nanoscale, however there is still a lack knowledge about the mechanisms at mesoscopic scale and as well as a comprehensive analysis of the electrical conductivity with the complexity of the material morphology.
Due to the high processability in water, we use graphene oxide (GO) as building blocks to produce complex structures in controlled way. We assemble single sheets with great precision into mesoscopic networks and macroscopic multi-layered films with tunable chemical and electrical properties by thermal reduction (RGO) (figure 1a).
We report a systematic study of charge transport properties of RGO assemblies with increasing network complexity. We find a general behaviour of the measured R(T). In all the cases we clearly distinguish two transport regimes characterised by a threshold temperature Tc depending on the chemical and the structural properties of the RGO assembly. For T<Tc, the charge transport is governed by ES-VRH, while for T>Tc a Power-law regime is observed. The experimental evidences indicate that the charge transport along the out-of-plane direction is (semi)metallic-like, similarly to the transport inside the sp2 domains. In the case of multi-layered films, the increase the number of overlapped RGO sheets allow to create alternative paths where charges can circumvent the in-plane defects by travelling out-of-plane, as schematically depicted in Figure 1b).

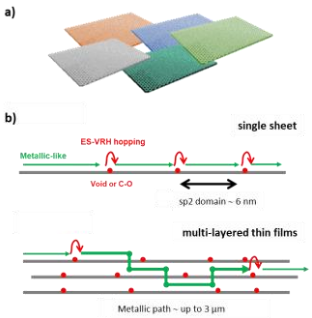

Figure 1: a) Scheme of RGO assembles. b) Scheme of the charge transport on single sheet and on thin film. The green arrow is the metallic like transport (no hopping) and the red arrow next to the border defects is the ES-VRH hopping.

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Organic field-effect transistor structures as a truly multifunctional platform: from light-emission to cell interfacing

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Abstract:
Organic light-emitting diodes (OLEDs) are a well-established class of devices for electroluminescence generation. Alternative driving schemes to generate electroluminescence from organic materials and to combine multiple functionalities, which offer fundamental advantages with respect to OLEDs, might impact a number of organic photonics applications including display technology and bio-sensing.
Here we discuss the concept of Organic Light-Emitting Transistors (OLETs) [1, 2, 3, 4, 5], highlight their specific electrical, optoelectronic and photonic characteristics with respect to OLEDs, and discuss their potential for practical applications.
In addition, we explore the use of organic transistor structures as a tool to stimulate and transduce the bioelectrical activity of neural cells. We demonstrate that transparent silicon-free transistor structures based on organic semiconductors are fully biocompatible and preserve the electrophysiological activity of both primary neural cells and non-excitable brain cells. On the one hand transparent Organic Cell Stimulating and Sensing Transistor (O-CST) [6, 7, 8] architecture fabricated with N, N'-ditridecylperylene-3,4,9,10-tetracarboxylic diimide (P13), provides bidirectional stimulation and recording of primary neurons. On the other hand, O-CST is able to elicit and monitor intracellular calcium signalling in primary rat neocortical astrocytes. These studies demonstrate that a properly designed organic transistor structure can be the base to develop bio-organic interfaces with unprecedented capabilities for the study of brain functions and for the therapy of brain pathologies.

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Field-modulated Graphene/Silicon Schottky diodes fabricated in a fully CMOS-compatible process line

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Abstract:

Since the publication of the first gate-controlled Graphene/Silicon (Gr/Si) Schottky barrier, also known as barristors, in 2012 by Yang et al [1], several works have appear trying to replicate the outstanding results of this publication. These include the replacement of silicon by other 2D materials such as $MoSe_2$ [5] and MoS_2 [6], or the use of oxides such as Ga_2O_3 [4] and Indium-Gallium-Zinc Oxide (IGZO) [5]. While the 2D heterostructures [2,3] were able to reproduce the high on/off ratio and current density, the required electric field to achieve this was over one order of magnitude larger in comparison with Yang et al. [1]. Moreover, the production of the 2D heterostructures [2,3] or the use of Ga_2O_3 [4] was through mechanical exfoliation in stark contrast to the high-yield CVD synthesis of Gr on Cu foils [1]. Conversely, the Gr/Metal Oxide heterostructure devices [5] were able to reach the high on/off ratios and current densities at comparable gate voltages using Cu-based graphene. Such fabrication procedure enabled these devices to be operational on a flexible substrate, however, the use of IGZO and ion gel as the gate dielectric represent an additional hurdle for Gr integration. In this work, we present the fabrication and characterization of field-modulated Gr/Si Schottky barrier vertical diodes produced at IHP's pilot line. While the fabricated barristors have significantly lower on/off ratios and current densities, the electric field required for the modulation amounts to only a few volts. Moreover, the Gr layer used was synthesized by CVD on CMOS-compatible Ge substrates, which completely removes the reported atomic residues left behind during the Cu-based Gr transfer. Furthermore, the I_{ds}/I_{gs} ratio, ß, from the Ge-based graphene devices can reach up to 10^8 which translates to a very low power control of the device. These results present further advances in the integration and implementation of Gr-based devices.

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Novel two-dimensional material device concepts through multi-scale simulations

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Abstract:
The advent of graphene and the related 2D materials has opened the possibility to boost the transistor performance, to conceive new devices and to engineer new materials with tailored properties. For these reasons, it is nowadays more and more urgent to have a robust and precise modeling framework able to incorporate the different materials and their possible combinations. Using a precise first-principle multi-scale approach we investigate multiple device configurations for digital applications. In particular, starting from Density Functional Theory (DFT) simulations [1], passing through the expression of the Hamiltonian in terms of Maximally Localized Wannier Functions [2] which feeds the open source device simulator NanoTCAD ViDES [3], and by means of Non-Equilibrium Green's Functions formalism, we inspect the operation of several device concepts. Specifically, we assess the performances of transistors made of a single 2D material, such as InSe [3], we present lateral heterostructures made of different phases of monolayer MoS2 [4] combining metallic and semiconducting phases to build up a Schottky diode and a lateral heterostructure FET. Then we explore different Noble TMDs materials, combining bilayer and monolayer crystals, as building block for nanoscale transistors [6]. Particular attention is devoted to Stanene, which has interesting features such as topological phases, localized edge states and magnetic phases when cut into zig-zag nanoribbon. We present two different tunnel field effect transistors (TFET) using thin Stanene nanoribbons: a proposal of a purely one-dimensional channel TFET device [7] and a spin filter device which exploits the possibility of independently tune the gap for spin up and spin down carriers with a lateral electric field [8].

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Influence of graphene particles on morphology and patterns on dewetting of thin polystyrene film

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Abstract:

A thin polymeric film has immense application in various fields like electronics, adhesive paints, lubricants, coatings, and biomedical applications. But in excessively thin polymeric films (< 100 nm) there is always a concern for the stability of the film. These ultrathin films are extremely unstable and tend to rupture and dewetting occurs leading to self-organization and pattern formation resulting in arrays of holes and droplets due to various reasons like spinodal decomposition, residual stress, van der Waals interaction, heterogeneous nucleation. In this paper we report the influence of graphene particles when embedded in a thin polymeric film. Graphene nanoparticles (85-150 nm) were used in a thin film (85-100 nm) to study the stability, dewetting and dynamics of the thin polystyrene film Graphene nanoparticles when inserted in thin polymeric film resulted in arresting the dewetting of the thin polymeric film and hence gaining the stability of these ultrathin polymeric films . These graphene particles not only arrested the dewetting but the dewetting patterns also deflected from its standard holes and droplets leading to formation of fingers and fractals. The different forces acting on the thin polymeric film like van der Waals, Laplace pressure and Marangoni flow along with the graphene nanoparticles gives way to different morphologies and patterns over thin film. The incorporation of graphene nanoparticles along with the formation of self-organized pattern due to instability over the thin liquid film gives rise to innovative morphologies for application in sensor, actuators, microelectronics, etc.

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Friday 7th

Effect of disorder on the magnetic stability of MoS_2 nanoribbons with zigzag edges

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Abstract:
Similar to graphene nanoribbons MoS_2 nanoribbons with zigzag edges also have magnetic properties according to DFT calculations [1]. This magnetism is associated with the metallic edge states where the edge sulfur atoms play an important role. However, investigating longer ribbons with large number of atoms is still computationally challenging.

In this work we provide a study of the magnetic properties of several nanometer long MoS_2 ribbon with zigzag edges. We applied tight-binding (TB) model in order to reproduce the electronic properties of the nanoribbons. By changing the TB parameters we were able to capture the metallic edge states of MoS_2 nanoribbons with their proper orbital characters providing us a simple starting point for the further inclusion of electron-electron effects. The magnetic calculations based on the Hubbard model predict low domain wall energies along the ribbon edges, which are also sensitive to the presence of edge disorder. Our results give an insight into the magnetic properties of MoS_2 nanoribbons in large scale systems and can also provide valuable information for spintronic applications.

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Atomic-scale Engineering of 2D Materials

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Abstract:
Despite the great promise of two-dimensional materials due to their exciting properties, they are not always directly suitable for applications. One way to tune the material properties is to manipulate the atomic structure using particle irradiation. However, as one might expect, this is challenging to do in the case of extremely thin materials, where careful control over the irradiation energy and solid understanding of the underlying atomic-scale phenomena are required. Despite the challenges, electron and ion irradiation have recently evolved into powerful techniques to manipulation the atomic structure of two-dimensional materials. At the same time, the recent advancements in aberration-corrected transmission electron microscopy both provide means to directly image the manipulated structures but also to fine tune them by inducing local structural changes and even to move defects and impurity atoms.
In this presentation, I will describe the advances in manipulating graphene with electron irradiation (e.g., Ref. [1]) and provide an overview of our latest results in using ion irradiation at a large energy scale to modify graphene and to implant foreign atoms into it [2], moving impurity atoms and defects at will (e.g., Refs. [3,4]), creating nanopores into graphene [5] and MoS_2, patterning graphene with gratings and two-dimensional amorphized areas [6,7] as well as other recent results.

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Introducing Functionalities in van der Waals materials by Lattice Modifications

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Abstract:
Edges, defects, and dopants in 2D transition metal dichalcogenides have been shown to give rise to chemical, electronic, and magnetic properties in these materials. To utilize the potential of these modifications a detailed understanding of their controlled formation and atomic scale properties is needed. In our group we aim at synthesizing 2D materials by molecular beam epitaxy and study approaches for controlled modifications by alloying, doping, one-dimensional modifications (edges or grain boundaries) or interfacing with dissimilar materials. In this talk we present our studies on the controlled formation of metallic mirror twin grain boundaries in $MoSe_2$ [1] or $MoTe_2$ [2] by incorporation of excess Mo into the lattice. Very high density of MTB networks can be obtained in $MoTe_2$ that effectively metallizes the material and thus may act as a metallic contact patch [3]. Such line defects may also increase electrocatalytic properties for hydrogen evolution reactions [4]. On a more fundamental level, we show that these 1D metallic grain boundaries host one dimensional electron gas and we present the first angle resolved photoemission (ARPES) studies of such line defects. These studies show evidence for the presence of Tomonaga-Luttinger Liquid behavior of 1D electron systems [5]. Finally, we show that other transition metals may also be incorporated into $MoTe_2$ and the incorporation of vanadium induces room temperature ferromagnetic ordering and thus is an example of a 2D dilute ferromagnetic semiconductor.

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Two-dimensional nanomaterials for artificial photosynthesis: Turning CO_2 into a valuable resource

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Abstract:

Photocatalytic CO_2 conversion to hydrocarbon fuels, the so-called solar fuels or artificial photosynthesis, making possible simultaneous solar energy harvesting and CO_2 reduction reaction (CO_2RR), is considered a killing two birds with one stone approach to solving the energy and environmental problems. However, the development of solar fuels has been hampered by the low photon-to-fuel conversion efficiency of the photocatalysts and lack of the product selectivity. Here, I would give a brief overview of our recent efforts in developing two- dimensional (2D) nanomaterials for CO_2RR. Notably, defect engineering (interstitial, vacancy, *etc.*) in 2D chalcogenides was found to be a viable method towards promising photocatalysts. Two cases will be illustrated: the carbon-doped SnS_2 nanosheets and single/few-layer MoS_2 with vacancies controlled by plasma treatment.

For the first case, the SnS_2-C nanosheets with a typical layer thickness of ~40 nm were synthesized using an L-cysteine-based hydrothermal process. Compared with undoped SnS_2, the interstitial carbon doping induced micro strain in the SnS_2 lattice, resulting in different photophysical properties. Density functional theory (DFT) calculations were performed for the formation energy, along with the CO_2 adsorption and dissociation on differently configured SnS_2-C for CO_2RR. The SnS_2-C exhibited a highly effective photocatalytic activity in gas phase with a photochemical quantum efficiency exceeding 0.7% under visible light, which is ~250 times higher than that of its undoped counterpart, and also a world-record high value reported for inorganic catalyst.

For the second case, the MoS_2 single to few layers were prepared by vapor transport deposition, followed by hydrogen plasma post-treatment. With increasing hydrogen plasma treatment time, we observed a trend of blue shift in the A_{1g} peak and red-shift in E_{2g} peak in their Raman spectra, implying creation of sulfur vacancies, of which the resultant stoichiometry ratio of Mo/S was further investigated by X-ray photoelectron spectroscopy (XPS). In addition, scanning tunneling microscopic images clearly supported that there were missing atoms in the MoS_2 layers after hydrogen plasma treatment. Productivity and selectivity of CO_2RR were found to be strongly dependent with the different Mo/S ratios of the MoS_2 single to few layers. The role and interplay of the defects and the hosting materials as well as their effects on CO_2RR, especially, the CO_2 adsorption behaviors by DFT simulation along with the near-ambient pressure XPS will be discussed in this presentation

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Layer number and photo-luminescence engineering of Molybdenite

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Abstract:
Among two dimensional materials beyond graphene, Molybdenum di-sulphide (molybdenite) being in the single layer phase a direct band gap semiconductor, is the prototypical system for optoelectronic applications. Its electronic and optical properties are tunable as a function of layer number and also by doping. We present here a systematic resonant Raman and photo-luminescence (PL) study of few and single layer mechanically exfoliated MOS_2. The mechanical exfoliation method is optimized and quantitatively rationalized [1]. We demonstrate that the electronic properties of the single and few layer MoS_2 can be tuned by creating sulphur vacancies via thermal induced sulphur desorption [2]. This leads to a controllable engineering of the photoluminescence response and tunes the relative intensity ratio of charged (trions) and neutral excitons. By comparing the PL response of single layer MoS_2 with thermally tuned sulphur vacancy concentration with resonant micro-Raman spectra we derive a self-consistent picture of the optical and electronic properties of defect engineered MoS_2 and propose evidences for the spatial symmetry of the exciton wave function. The effects of thermal annealing are also discussed in relation to post exfoliation layer engineering and of the gas sensing response of the material [3].

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Bent-Lattice Nanostructure in Crystallized Amorphous Films: from Transrotational Nanoengineering to Novel Amorphous Models

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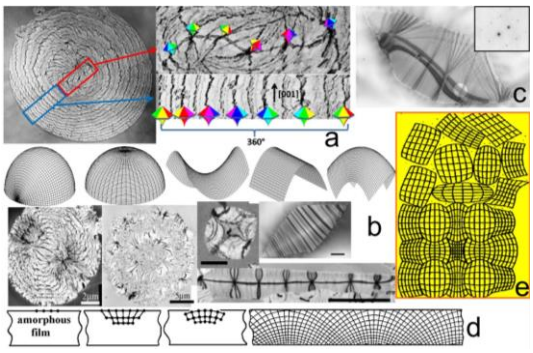
Abstract:
Exotic thin crystals with unexpected **transrotational nano**structures [1] have been discovered by transmission electron microscopy (TEM) for crystal growth in thin (10-100 nm) amorphous films of different chemical nature (oxides, chalcogenides, metals) prepared by various methods. TEM bend-contour method [2] used is combined with SA electron diffraction. HREM, AFM and optical microinterferometry were used in due cases (preferentially for correlative microscopy). The unusual phenomenon can be observed ***in situ*** in TEM column during local e-beam heating or annealing: regular internal bending of crystal lattice planes in a growing crystal (dislocation independent), Fig.1a-b. Such **transrotation** (**trans**lation of the unit cell is complicated by small **rotation** realized round an axis lying in the film plane) can result in strong regular lattice orientation gradients (up to 300°/μm) of different topology: cylindrical, ellipsoidal, toroidal, saddle, etc., Fig.1b The possible mechanisms of the phenomenon are discussed. Fig.1d. Initial amorphous state and surface nucleation of the crystal growth are most essential factors. The last fact accompanied by anisotropy of crystal growth rate and obvious tendency for regular change of interatomic distances of the crystal propagating from the surface layers inside the bulk material resembles specific epitaxy, "vacuum epitaxy". The **transrotation** phenomenon is the basis for novel lattice- rotation nanoengineering of functional, smart thin-film materials suitable also for strain nanoengineering. Transrotational micro crystals have been eventually recognized by different authors in some thin film materials vital in applications, e.g. phase change materials (PCM) for memory [3-5]. New nanocrystalline models of amorphous state are proposed: fine-grained structures with lattice curvature, Fig.1e. Thus different transrotational lattice topology inside fine crystal grains in the static model corresponds to different amorphous structures. Going to 3D clusters of positive/negative curvature and dynamics we propose the hypothesis of "dilatons" and "contractons" pulsating or/and circulating in amorphous film.



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Non-Covalent Functionalization of Monolayer MoS_2 –Tuning the Electronic Structure

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Abstract:

Transition metal dichalcogenides (TMDs), such as e.g. MoS_2, WSe_2 represent a large family of layered 2D materials, which cover a broad variety of electronic, optical and mechanical properties and therefore can serve as the functional part in various microelectronic devices.

The diverse properties are often determined by the method of fabrication, which can be liquid phase or mechanical exfoliation, thermally assisted conversion (TAC) or chemical vapour deposition (CVD). Due to their monolayer nature the properties of 2D materials strongly depend on the environment, which makes control and modification of the surface chemistry a powerful tool to obtain changes in the materials behaviour. Functionalization of the surface leads to doping via charge transfer, resulting in tunable electrical properties, which can be exploited in electrical devices such as diodes, FETs, chemiresistors or ChemFETs.

The approach discussed in this contribution includes physisorption of organic molecules onto relatively large-scale monolayer CVD grown MoS_2 films, forming self-assembled monolayers (SAMs) through van der Waals interactions. In particular we focus on the on-chip non-covalent functionalization by organic species of the class of perylene bisimide molecules and study the effect on the electronic properties of MoS_2 with first-principle FET structures. Additionally investigations by Raman spectroscopy, XPS, and scanning probe techniques on the hybrid inorganic-organic structures have been carried out.

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Lithographic band structure engineering of graphene

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Abstract:
Two-dimensional materials such as graphene allow direct access to the entirety of atoms constituting the crystal. While this makes shaping by lithography particularly attractive as a tool for band structure engineering through quantum confinement effects, edge disorder and contamination have so far limited progress towards experimental realisation.

In this talk, we show work on a superlattice of holes (12-15 nm minimum feature sizes) etched in graphene encapsulated by hexagonal boron nitride, which results in profound effects on the band structure and the resulting quantum transport [1].
Through the high-quality lithographic patterning of the graphene, we achieve ballistic transport while opening a bandgap on the order of 0.15 eV. In magnetotransport measurements, we observe a regime that is distinctly different from the characteristic Landau fan of graphene, and further, observe that the bandgap can be continuously turned off by increasing the magnetic field strength. The measurements are accurately described by transport simulations and analytical calculations.

Finally, we observe strong indications that the lithographically engineered band structure at the main Dirac point is cloned to a satellite peak that appears due to moiré interactions between the graphene and the encapsulating material. Band structure design in two-dimensional materials by top-down patterning enables the realisation of many exciting predictions and opportunities such as spin qubits [2], valleytronics [3] and waveguides [4].

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Scattering Theory of Graphene Grain Boundaries

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Abstract:
The implementation of graphene-based electronics requires fabrication processes that are able to cover large device areas, since the exfoliation method is not compatible with industrial applications. The chemical vapor deposition of large-area graphene represents a suitable solution; however, it has an important drawback of producing polycrystalline graphene with the formation of grain boundaries, which are responsible for the limitation of the device's performance. With these motivations, we formulate a theoretical model of a single-layer graphene grain boundary by generalizing the graphene Dirac Hamiltonian model. The model only includes the long-wavelength regime of the charge carrier transport, which provides the main contribution to the device conductance. Using symmetry-based arguments deduced from the current conservation law, we derive unconventional boundary conditions characterizing the grain boundary physics and analyze their implications on the transport properties of the system. Angle resolved quantities, such as the transmission probability, are studied within the scattering matrix approach. The conditions for the existence of preferential transmission directions are studied in relation with the grain boundary properties. The proposed theory provides a phenomenological model to study grain boundary physics within the scattering approach, and represents per se an important enrichment of the scattering theory of polycrystalline graphene. Moreover, the outcomes of the theory [1] can contribute to understanding and limiting the detrimental effects of graphene grain boundaries, while also providing a benchmark for more elaborate techniques.

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Manipulation of epitaxial graphene towards novel 2D materials

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Abstract:

Integration of epitaxial graphene with SiC can bridge the excellent intrinsic properties of the semiconductor and semimetal, enabling novel high-performance devices. Furthermore, interfacing this combined system with different metals, may allow tunability of electronic and optical properties of the designed 2D materials. We identify the epitaxial graphene on SiC as the ideal platform to template their growth. Taking advantage of the maturity of our epitaxial graphene approach we have been able to address different growth scenarios in order to tailor the properties of the interfaces in this unique material system - the reconstructed carbon rich SiC interface (buffer layer) and the first graphene layer. We prepared graphene templates on 4H-SiC by thermal decomposition followed by exposure to hydrogen flow at different temperatures. We anticipate that the interface site and structure will guide the formation of 2D materials with desired functionality, particularly metal-on-graphene and metal-under-graphene hybrids. We focus on the impact and respective manipulation of the graphene template by in-situ and ex-situ treatments in order to extend our knowledge and growth capability towards attaining full control over growth of large area 2D metal layers and nanoclusters with given properties for novel application, e.g. sensing, catalysis, contacts, etc. As a first step, we study the effect of hydrogen intercalation which is the most viable way to decouple the buffer layer from the SiC substrate and allow a confined space for synthesis of nanophases. Although hydrogen intercalation of graphene has been previously studied, we have found new relationships pointing to the process optimization. We have employed in depth analysis of Raman spectra, C-AFM measurements and DFT modelling. The reduction of the intercalation temperature from 1100˚C to 900˚C caused a reduction of the compressive strain and the degree of strain fluctuations. We ascribe such phenomenon to a strain relaxation due to local enhancement of the carrier density. The combined application of micro-Raman mapping and C-AFM allowed to investigate in detail the homogeneity of hydrogen intercalation of buffer layers on 4H-SiC(0001). Our results give deep insights into the nature of the physical processes underlying the structural changes of the buffer layer upon hydrogen intercalation. As a next step metals are deposited on the templates and the observed effects like layered growth and SERS are discussed.

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Composition and Electronic Properties of $PtSe_2$ and other Transition-Metal Dichalcogenides Investigated by Photoelectron Spectroscopy

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Abstract:

Platinumdiselenide ($PtSe_2$) is a group-ten transition-metal dichalcogenide (TMD) with a number of interesting properties. With its thickness decreasing to a few monolayers, $PtSe_2$ shows a transition from semimetal to semiconductor. With a bandgap in the infrared region, potential applications of the semiconducting 2D layer range from gas sensing to microelectronics and – due to its high piezoresistivity – even micromechanics. Moreover, the material can be synthesized at low temperatures using thermally assisted conversion (TAC), which makes it suitable for back-end of line processes and - what is also important for applications - it is stable in ambient.

The composition of TAC-grown $PtSe_2$ films was studied using X-ray Photoelectron Spectroscopy (XPS) and Ultraviolet Photoelectron Spectroscopy (UPS) depending on the depth inside the layer. Due to the few-layer thickness of the material, ultra-shallow depth profiling with monolayer resolution is required. Not only the $PtSe_2$ film itself, but also the substrate interface is of special interest due to its effect on the electronic properties of thin films. Depth profiling results were compared to TOF-SIMS measurements of the same layers. At the surface, UPS was employed for work function measurement. Additionally, work function values were verified by Kelvin Probe measurements. The techniques shown here can also be applied to other TMDs, like MoS_2.

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Spectroscopy of inelastic processes in quantum Hall edge channels: a possible resolution to the missing energy problem

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Abstract:

Quantum Hall edge channels offer an efficient and controllable platform to study quantum transport in one dimension. Such channels are a prospective tool for the efficient transfer of quantum information at the nanoscale, and play a vital role in exposing intriguing physics. Electric current along the edge carries energy and heat leading to inelastic scattering, which may impede coherent transport. Several experiments attempting to probe the concomitant energy redistribution along the edge reported energy loss via unknown mechanisms of inelastic scattering. Here we employ quantum dots to inject and extract electrons at specific energies, to spectrally analyze inelastic scattering inside quantum Hall edge channels. We show that the "missing energy" puzzle can be untangled by incorporating non-local Auger-like processes, in which energy is redistributed between spatially separate parts of the sample. Our theoretical analysis, accounting for the experimental results, challenges common-wisdom analyses which ignore such non-local decay channels.

Entanglement manipulation in hybrid TI-S nano-devices

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Abstract:
We discuss the supercurrent of hybrid topological Josephson junction done with two superposed layer of topological insulator (see Fig.1) which allows local (LAR) and crossed (CAR) Andreev reflections with the s-wave leads [1]. We show that by simply applying realistic external potentials such as gate potentials or magnetic flux to the junction one can uniquely affect the dissipationless current. In particular we showed that local gating, thanks to its symmetry with time-reversal, is able to manipulate the spin symmetry of non-local Cooper pairs from singlet to triplet. We establish both analytically and numerically the connection between the Josephson current-phase relationship and the entanglement manipulation. We investigate notable limits, such as the single-shot regime, which clearly demonstrate that entanglement symmetry manipulation can be identified in the critical current. Finally we discuss the universal behavior of the critical current, how it depends on the amplitude ratio between the CAR and LAR processes and on the external potential manipulations. The proposed setup and the simple signature in the dependence from external potentials are expected to be experimental accessible with the measurement of the critical currents which one the most basic characterization of a Josephson junctions.

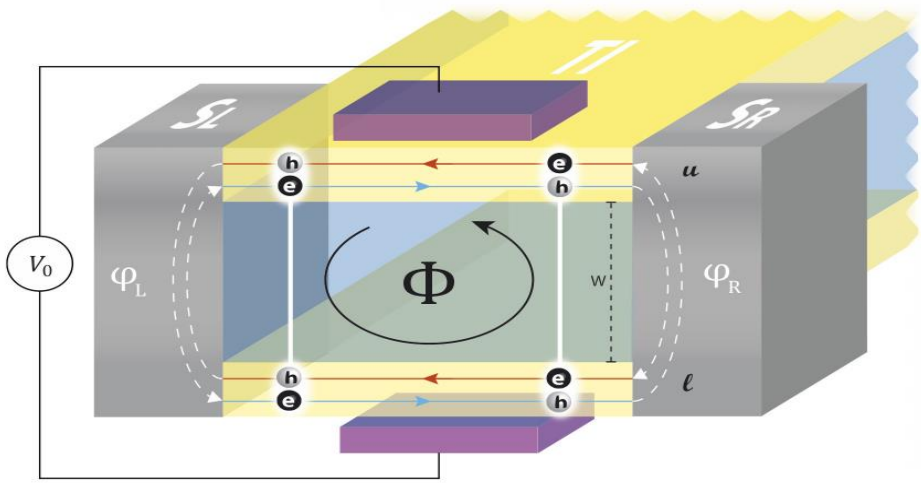

Fig. 1: Double TI Josephson junction and external potentials.

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Strong proximity Josephson coupling in heterojunctions of 2D materials

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Abstract:
Realization of proximity coupling in Josephson junctions, incorporating various two-dimensional (2D) van der Waals materials including graphene, has recently attracted much research interest. In this talk, I will focus on the short-ballistic (SB) strong Josephson coupling realized in vertical and planar proximity Josephson junctions with mono-layer graphene as the thin normal-conducting spacer. The short-ballistic junction characteristics provide highly robust coherent states to be utilized for possible quantum-device applications. Here, for vertical graphene Josephson junctions (GJJs), the SB strong proximity coupling is realized by shortening the channel length down to the thickness of mono-layer graphene between two superconducting-layer electrodes. For planar GJJs, the SB strong coupling is realized via the ballistic conducting channel of a boron-nitride-encapsulated graphene layer. If time allows, I will also discuss how the Josephson effect is utilized to study fundamental material properties such as the robust surface conduction in a topological insulator and the edge conduction in 2D materials such as quantum spin Hall insulators and graphene. For details on the topics, one may refer to Ref. [1].

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Atomic-scale spin dynamics

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Abstract:
Spin dynamics are particularly relevant in nanoscale materials, where they give rise to exciting phenomena such as slow relaxation of magnetization or quantum critical behavior. Accessing these dynamics on their intrinsic atomic length and time scales is an important step towards an understanding of their underlying quantum behavior. Scanning tunneling microscopy experiments with high frequency signals [1, 2] both give access to the spin lifetime of nanostructures and provide real space atomic-scale resolution.
We show how using pulsed signals, all-electronic pump-probe experiments can be performed, which allow nanosecond scale dynamics to be resolved. These measurements are highly sensitive to the spin's interaction with its local environment. Taking advantage of this sensitivity, remote sensing of atomic-scale spin systems was demonstrated via a newly identified magnetic coupling mechanism on the copper nitride surface.
To go beyond the nanosecond scale, we find that broadband noise spectroscopy allows the identification of picosecond fluctuations of an individual atom. These fluctuations reveal that small variations in local topography have a significant impact on the dynamics of the individual atom.
Combining local measurement of spin dynamics with atom manipulation techniques makes it possible to explore the emergence of collective states in coupled quantum systems in a highly controlled environment.

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Spintronics at the interface

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Abstract:
The interface between materials can be considered as the ultimate spintronics device, not only in terms of miniaturization but also to unlock unique design pos- sibilities and new physical properties which are unattainable in the individual bulk materials. As device dimensions are constantly shrinking, understanding the physical properties emerging at interfaces is crucial to exploit them for applications.
Graphene and magnetoelectric multiferroics are promising materials for spin- tronic devices with high performance and low energy consumption. We combine the features of both materials by investigating from first principles and Monte Carlo simulations the interface between graphene and $BaMnO_3$, a magneto-electric multiferroic. We show [1] that electron charge is transferred across the interface and magnetization is induced in the graphene sheet due to the strong interaction between C and Mn. A remarkably large proximity induced spin splitting of the Dirac cones ($\sim$ 300 meV) is achieved and doping can make the high-mobility region of the electronic bands experimentally accessible.
Spin-Orbit Coupling calculations reveal that graphene deeply affects the magnetic state of the substrate, down to several layers below the interface, by inducing an overall magnetic softening, and switching the in-plane magnetic ordering from anti- to ferromagnetic. The graphene-$BaMnO_3$ system presents a Rashba gap 300 times larger than in pristine graphene, leading to a new flavor of Quantum Anomalous Hall effect (QAHE), a hybrid QAHE, characterized by the coexistence of metallic and topological insulating states. These findings could be exploited to fabricate novel devices that use graphene to control the magnetic configuration of a substrate [2].

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Stability and lifetime of magnetic skyrmions from density functional theory

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Abstract:
I will talk about our ongoing efforts to understand and predict stability and lifetime of spin textures with topological charge, also called magnetic skyrmions. Magnetic skyrmions hold great promise as a basis for a new type of information technology. In particular, information flow can be associated with metastable skyrmions driven along a magnetic strip, as suggested in skyrmion racetrack schemes. It has been demonstrated that skyrmions are sensitive to controlled external stimuli such as electric current, which is beneficial for efficient, low power data processing. For such a technology to be viable, however, the skyrmion lifetime, τ, is an essential quantity. We combine an atomistic spin Hamiltonian parametrized from density functional theory with harmonic transition state theory to compute the lifetime of skyrmions. We find that thermal stability of magnetic skyrmions can be strongly affected by entropic effects and the frustration of long range exchange interactions. Our results open the door for predictive simulations, free from empirical parameters, to aid the design of skyrmion-based information technology.

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Mechanisms of photoconductivity in atomically thin InSe and GaSe

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Abstract:
The layered III-VIA semiconductors family has attracted large interest recently and many applications based on these materials have been reported, such as single-photon emitters working at room temperature and strong optical non-linearity [1]. In this talk I will discuss our recent experimental efforts in explaining the mechanisms behind the photocurrent generation in photodetectors based on GaSe and InSe. We find that both materials react with air and we observe a change in the responsivity and speed of operation of the devices. The effects can be described by a a competition between photogating and photoconductive effect [2, 3]. These observations can be explained by the presence of electronically active traps in the system, mostly associated with selenium vacancies. These can interact with the oxygen present in the air and influence the generation of photocurrent. Interestingly while in GaSe the interaction with air leads to the failure of devices in a few days, in InSe the degradation process is a self-limiting process and the devices are stable in air for months.

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Optical probes of defects in lead halide perovskites

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Abstract:
Lead halide perovskites (such as $CH_3NH_3PbI_3$) have recently attracted huge interest, with potential use as a solution processable semiconductor for photovoltaics, LEDs and lasers. Recent publications have increasingly focused on the nature and role of defects, both for their part in determining intrinsic material photophysics, and with regards to device instability and degradation. We will present a series of results describing applications of time-resolved and steady-state optical spectroscopy to the study of defects in these materials.

Instabilities are manifested as light-induced ion migration and segregation. They can eventually lead to material degradation under prolonged exposure to light. At the same time discordant reports discuss about the beneficial role of ion migration under illumination, leading to defect healing. Thus, understanding the photo- chemical and physical processes behind such phenomena and eventually mastering them is a fundamental step towards a solid exploitation of perovskites in optoelectronic devices.

By combining photoluminescence measurements under controlled conditions with ab initio simulations we reveal that photo-instabilities are related to both light-induced formation and annihilation of defects acting as carrier trap states. These phenomena coexist and compete, and furthermore can be controlled, guiding development of more efficient and stable halide perovskite devices.

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Defects, interlayer coupling and Fermi resonance in 2D materials

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Abstract:
Van der Waals heterostructures give access to a wide variety of new phenomena that emerge due to the combination of layered materials with different properties.
One of the key to engineers the properties of 2D materials could be in our ability to alter their structure in a controllable way. Different methods are possible: functionalization, intercalation, inducing defects etc. Whatever the chosen method the consequences is a strong modification of their structure and thus on their electronic and vibrational properties. All these effects can be probed efficiently by optical phonons.

In this work we will try to unravel the structural modification induced by defects in the case of graphene and MoS_2 . In the case of few- and single-layer MoS2 hosting substantial defects densities, these defects are thought to influence the doping level, the crystal structure, and the binding of electron–hole pairs. We disentangle the concomitant spectroscopic expression of all three effects and identify to what extent they are intrinsic to the material or extrinsic to it. We discover a defect-bound state having a low binding energy of 20 meV that does not appear sensitive to strain and doping, unlike charged excitons. Conversely, the defect does not significantly dope or strain MoS_2 [1].

We also show here that due to an enhanced interaction cross section in such structure, made of molybdenum disulphide and boron nitride, electron-hole pairs can be generated by incident electrons and give rise to cathodoluminescence. Using Raman spectroscopy and photoluminescence, we show that low energy electron beam irradiation can nevertheless cause irreversible structural damages in molybdenum disulphide. A correlation between molybdenum disulphide/boron nitride coupling and the defect creation is established. Our work demonstrates that cathodoluminescence is powerful tool images the electronic properties in van der Waals heterostructures at the nanometer scale.
In the case of graphene, we report the observation of an intense anomalous peak in the Raman spectrum in specific growth conditions that cannot be attribute to structural defects. In fact, bombardment with an electron beam demonstrates that this new peak is clearly distinct from the well-studied D' peak appearing as defects are created in graphene [3].

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Bottom-up synthesis of atomically precise graphene quantum dots

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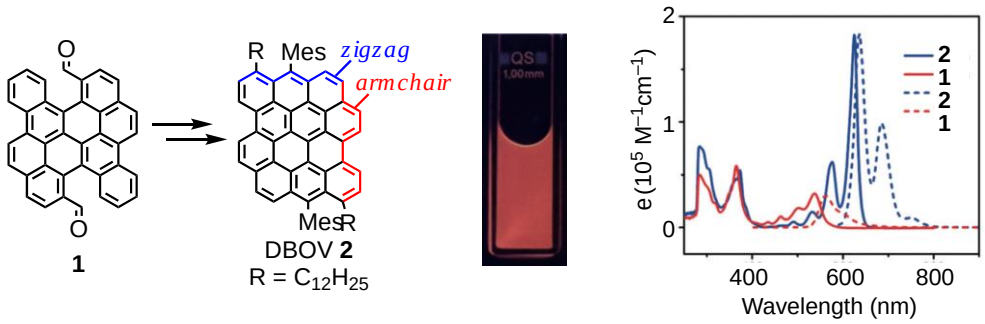
Abstract:
Whereas graphene demonstrate exceptional electronic and mechanical properties, its lack of bandgap prohibits its applications as an active semiconductor material [1]. In contrast, graphene nanostructures such as graphene quantum dots (GQDs) and graphene nanoribbons (GNRs) possess non-zero energy gaps due to quantum confinement effect, and are promising for nanoelectronic and (opto)electronic applications [1]. The properties of such nanoscale graphenes are critically dependent on their size, morphology, and edge configuration, which makes it essential to precisely control their chemical structures. Although, the required precision cannot be achieved by "top-down" fabrication methods such as "cutting" of graphene, bottom-up chemical synthesis can achieve atomically precise GQDs and GNRs [1]. We have recently developed a synthesis of dibenzo[*hi*,*st*]ovalene (DBOV **2**) as highly luminescent and stable GQD, starting from another GQD **1** [2]. DBOV with a combination of zigzag and armchair edges demonstrated strong red emission with quantum yield of ~80% and stimulated emission [2-4], rendering it promising for applications in light-emitting devices. We have further achieved precise edge functionalization of DBOV, allowing for introduction of different substituents and modulation of the optical properties [5]. We have also obtained water-soluble DBOV, allowing for application in bioimaging.



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Self-assembling at molecular resolution: the power of organizing the unorganized

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Abstract:
Self-assembling is a fascinating phenomenon observed in nearly all life processes. It relies on precise non-covalent interactions, which act on extraordinarily diverse scales of time, size, and complexity while preserving an exceptional level of specificity. This have motivated researchers from several areas of nano-biotechnology to mimic and engineer assemblies. Most often, their design takes its inspiration or is informed by features of naturally occurring assemblies, and it has promoted the growth of predictive computational models enabling the design of novel supramolecular materials. Achieving full control over self-assembled complexes with target architectures and specific functionalities is still one of the open challenges in the field.
In this contribution, several examples of self-assembling systems recently studied by us will be illustrated. These include functionalized metal nanoparticles, block-copolymers, and self-assembling short peptides for nano-bio applications. The combination of molecular models obtained via computational techniques coupled with experimental evidences helped in providing new insights into the molecular forces driving the behavior of these collective materials, supporting the design of novel optimized nanosystems.

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Fabrication and characterization of nanomaterial-based sensor devices using solution printing method

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Abstract:

Near future, we will get super smart society (Society 5.0) which a lot of data are gotten form our physical society by IoT technologies with all sensing systems. The big-data in cyber space are optimized and added additional values through AI and ICT technologies, and feedback actionable information to us in the physical space. This concept is calling cyber physical systems (CPS). The CPS will solve all social issues, and develop new economical services and industries through improving productivity.

Sensing devices such as gas sensor, thermistor, and pyroelectric sensor are very important of the IoT technologies in CPS. The sensor devices have to develop not only more good sensing property, but also cost effective fabrication process and low energy consumption during running. The sensors productivity have been developing with enhanced sensing properties. Printed electronics (PEs) with solution chemical method is one of the much attention technology intend to next generation electronics device manufacturing for cost effective and mass product such as high-throughput, large-scale, and resource saving over conventional process.

In the previous study of our group, metal nano material and oxide nanostructure arrays have been successfully synthesized via solution method. Here, we are demonstrating fabrication of electronic sensor devices by printing method using our nano-materials, e.g. MoO_x, TiO_x nano-stracture, and Cu, Ag nano-wires (NWs).

Gas sensor devices using the fine metal oxide nano-stracture fabricate for volatile organic compounds (VOC) gas with a simple solution MOD with printed coating process. The gas sensor shows good performance with response time and complete recovery, as well as various selectivity of VOC gas at 573 K. Thermistor (heater) devices are demonstrated good electrical and thermal stability duling thermal and mecanical cycle testing used stretchable transparent conductive electrode with Cu@Ag alloy NWs. These results are suggested that the PE technologies with nanomaterials may greatly contribute to the manufacturing process and reliability of next generation electronics devices in Society 5.0.

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Laser ablation synthesis in solution and nanoalloys: a fruitful combination

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Abstract:

Laser ablation of solid targets in liquid environment allows the production of nanoparticles (NPs) with peculiar surface chemistry and a large variety of compositions, included metastable phases and nanocomposites, all by the same self standing and simple set up [1]. Currently, several efforts are undergoing to improve the control on laser generated nanomaterials and to precisely understand the formation mechanism of nanoparticles. In this context, nanoalloys of noble metals and transition metals are a useful case-study, because of the different chemical transformations observed in different chemical elements subjected to the same laser ablation process [2]. On the other hand, these noble metal nanoalloys consist of metastable phases hardly achievable by other synthetic approaches, and have multiple functions which are exploitable for plasmonics, surface enhanced Raman scattering (SERS), catalysis and nanomedicine [3].

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Advances in Properties and Synthesis of MoS_2 and WS_2 nanotubes

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Abstract:
The discovery of inorganic nanotubes (INT) of layered transition metal dichalcogenides (MoS_2 and WS_2) more than two decades ago opened the new research field in the solid state chemistry and in nanomaterials science. However, wide investigation of their properties and applications requires the preparation of pure phase powders and, therefore, detail understanding of their growth mechnism.
Indeed, recent study of WS_2 multiwall nanotubes' (MWINT) synthesis via solid-gas reaction resulted in pure phase INTs production of 15 g/week and suggested their simple scaling up. The obtained nanotubes are of 30–120 nm in diameter and 2- 20 micron in length, of perfect crystallinity and needle-like morphology.
In addition, we have demonstrated that single- to triple-wall WS_2 nanotubes (SWINT), of 3-7 nm in diameter and 20-200 nm in length, can be produced by high-power plasma irradiation of big MWINT-WS_2 nanotubes. Being of single to few-layers wall-width these nanotubes promise to be of unusual electro-optical characteristics, which are under study nowadays. Initial results on cathodoluminescence (CL) observation in these nanoparticles confirm quantum confinment effect in single wall few-nm in diameter tubes.
Very similar in their properties, the MoS_2 and WS_2 compounds demonstrate, however, significantly different behavior during their synthesis from corresponding oxides through solid-gas high temperature reaction. Finally (25 years after heir discovery), we can report on the reproducible, catalyst free and aspect ratio controlled synthesis of MoS_2 inorganic nanotubes (INT) from molybdenum oxide. INT of MoS_2 are both 40% lighter and 40% stronger compared to the analogous WS_2 nanoparticles and hence more beneficial for tribological and composite applications. Being semiconductors, both MoS_2 and WS_2 nanotubes are good candidates for photovoltaics and optoelectronics.
The availability of MWINT-WS_2 in large amounts led to extensive investigation of their properties suggesting numerous applications. The results on BPVE (bulk photovoltaic effect), Raman spectroscopy, hydrogen storage and polymer stengthening based on these nanotubes will be presented.

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Nanocrystal dimers: fabrication and properties

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Abstract:

A growing interest has recently been devoted to the synthesis and organization of nanocrystal (NCs) and nanostructured materials. In this dimensional regime, the electronic structures can be tuned by varying the physical size of the crystal, leading to new phenomena, as surface plasmon resonance in metal nanoparticles and size-dependent optical transitions in semiconductor quantum dots, opening interesting opportunities for device applications. NCs synthesized by solution chemistry approaches represent potential building blocks for inexpensive manufacturing of low cost and large area devices. The synthesis, performed in the presence of surfactants as stabilizers, allows to control in a reproducible manner size, shape and crystalline phase of the nano-objects. Accordingly, the choice of the organic ligands depends on their capability to coordinate the surface of the nanoparticles during the growth. Currently, intensive research has focused on the fabrication of NC based organized meso-structures in solid state, which have shown new and interesting properties due to the collective interactions of nanoparticles. In principle, the simplest way to investigate the new properties deriving from the NC coupling in complex nanostructures is probably to fabricate dimers obtained by combining only two nano-objects, varying their composition or dimensions. However, the preparation of chemically stable dimers in solution is not trivial. Here we present recent results concerning the realization of dimers based on luminescent quantum dots, obtained in solution. Dimers of CdSe quantum dots of the same size (homodimers) or of two different sizes (heterodimers) were fabricated by using dithiols as bifunctional linkers, bridging the two nanoparticles and morphological (high resolution TEM) and spectroscopic (UV-Vis absorbance, stationary and time resolved photoluminescence spectroscopy) characterized. The use of dithiol binders with diverse alkyl chain length allowed to control and to modulate the interparticle distance in the nanometric and subnanometric range. The comprehensive spectroscopic investigation of the dimers pointed out coupling effects that are not rationalizable just as a FRET mechanism. Such effects are reasonably attributed to the coupling between the delocalized electronic wave functions on the two quantum dots. The preparative approach can be extended to colloidal nanocrystals of different size and composition, giving rise to a plethora of original and unexpected phenomena.

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Saturday 8th

Amorphous and crystalline gallium oxide thin films by atomic layer deposition

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Abstract:

Gallium oxide has attracted renewed interest as an ultrawide band-gap transparent semiconductor. Ga_2O_3 crystallizes in five different polymorphs, among which the monoclinic phase is the stable phase at room temperature and atmospheric pressure. -Ga_2O_3 films are expected to be highly suitable for various applications such as high temperature and ultra-high-voltage electronics, photon detectors, gas sensors as well as thin tunneling barriers in various devices.

In this presentation, we will focus on the growth and on the characterization of gallium oxide thin films by plasma-enhanced atomic layer deposition (PE-ALD). The films were grown on silicon substrates starting with trimethyl gallium as the Ga precursor and oxygen plasma as the oxidizing agent. Various surface treatments prior to deposition and various processing parameters were investigated. In situ ellipsometry was used to determine the average growth rate while varying the growth parameters. X-ray photoelectron spectroscopy and X-ray diffraction were performed to determine the bonds and the crystalline structure of the materials. In a temperature range of 100-360ºC, the growth per cycle (GPC) is of ~ 0.67-0.70Å/cycle – in good agreement with previous reports (1,2) - and the films are amorphous. Uniform amorphous gallium oxide films are obtained on 200 mm Si wafers with a change in thickness and in refractive index over the full area of 1.4% and 0.2% respectively (for a nominal thickness of ~ 28 nm). After gallium oxide deposition, the samples were annealed in N_2 atmosphere in a tubular furnace or by rapid thermal processing (RTP). While the Ga valence is comprised between 1 and 2 for as deposited films, Ga^{3+} oxidizing state is revealed by XPS after annealing. The leakage currents were lowered by adjusting the O_2 plasma duration and the post-deposition annealing conditions. The electrical properties of the amorphous and crystalline phases will be discussed.

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Graphene Technology: synthesis, characterization and reliability-driventechnological device integration

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Abstract:
Graphene fascinating properties hold promises for a great technological impact [1]. Nevertheless, to allow for a real exploiting of their extraordinary properties, a complete controlof the fabrication steps of graphene-based devices is mandatory. In this contribution we will show an integrated approach for the integration of graphene membranes in state-of-the-arttechnological processes and for the exploitation of their properties in an applicative framework.
Our approach starts from the careful control of the synthesis parameters of the CVD growth ofgraphene membranes, as well as of their structural and functional properties. It moves then to the definition of tailored transfer processes leading to the integration of graphene membranesin a wide class of functional substrates (technological surfaces, glass, plastic and polymericflexible substrates), as well as of their surface functionalization, to provide the control ofphysical and chemical properties over large area, typically mandatory in the device's fabrication processes. [2-5]. Final step is the definition of the complete set of technological processing steps needed toachieve a full integrability of the membranes within the processes of fabrication of micromachined devices. To this aim, since the integration of graphene hybrid devices in silicon CMOS requires high reliability and yield, the full development is supported by the Design forReliability approach which will address graphene-based electronic devices to really enter themarket in the near future, with the maturity level requested by IC technology. More in detail, this is achieved through three main blocks: 1) definition of the requirements for large-scalegraphene integration; 2) identification of critical graphene processes for the integration andtheir optimization; 3) identification of measurement methodologies, standards, data and modelsfor the development of a reliable fabrication process, an accurate process control and theoptimization of the processes.

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Preparation of Graphene Oxide-Quantum Dot Hybrids for the Detection of Ascorbic Acid

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Abstract:
Water-soluble fluorescent carboxyl-functionalized CdSe-ZnS quantum dots (QDs) were immobilized on graphene oxide (GO) and used for sensitive detection of ascorbic acid in aqueous solutions. QDs were attached to the surface of graphene oxide using the EDC/NHS-sulfo coupling reaction. Ascorbic acid is known as an antioxidant. It plays a crucial role in health maintenance, bio synthetic pathways such as formation of collagen and regulates immune system.
The photoluminescence (PL) intensity of as-prepared GO-QD hybrids in water was quenched by ascorbic acid at ambient temperature. Based on this photoluminescence quenching phenomenon, a simple, rapid, and sensitive procedure is developed. The PL intensity of GO-QDs was sensitive to pH values and stable over a period of 4 days. The PL quenching efficiency shows a good linear relation with AA concentration with a detection limit of 568 pM and a correlation coefficient (R2) of 0.9941. This shows that simple and sensitive detection of AA at the picomolar level is possible by using GO-QDs.

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Plasma-assisted Synthesis and Modification of Carbon Nanowalls for Emerging Applications

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Abstract:

Carbon nanowalls (CNWs) are one of carbon nano-materials, which consist of self-assembled and multi-layered graphene sheets standing vertically on the substrate. Owing to their three-dimensional nanostructures, they have the high aspect ratio over 100 and high specific surface area. In addition to such the unique morphologies, they also have unique and excellent electrical properties. Therefore, they have attracted much attention to be applied to various types of devices, such as electrical devices, electrochemical sensors, biosensors, and so forth, and scaffold of cell culturing. To realize such the applications, not only control of their morphology, but also chemisorbed species on their surfaces were important. Recently, establishing a radical-injection plasma-enhanced chemical vapor deposition (RI-PECVD) system, we realized highly reproducible growth of CNWs and, controls of their morphology and semiconducting properties. According to absolute density measurements of radicals by vacuum ultraviolet absorption, with increasing the density of hydrogen radical, the density and growth rate of CNWs decreased owing to its etching effects on growth surfaces. Therefore, hydrogen radical is one of important factors to determine the density and growth rate of the CNWs. An ion bombardment is also important for the nucleation of nanographene at the early stage of CNWs growth.

High density over 10^{13} cm^{-2} Pt nanoparticles can be supported on whole surface area of the CNWs by supercritical fluid method. Such the Pt nanoparticles-supported CNWs (Pt-CNWs) are very effective as a catalyst electrode in fuel cells. They have high durability and long-life time in the cycling of start-stop operations with high voltage applying. On the other hand, Pt-CNWs is also a good sensing electrode. Using the Pt-CNWs electrodes, mere 50 nM of H_2O_2 can be detected in PBS. The CNWs also exhibit interesting properties as a cell culture scaffold. The cell culturing rates of HeLa cells were significantly dependent on the CNW densities, although the surface wettability of the CNWs was not significantly dependent. On the other hand, Morphological changes of the cells were not significantly dependent on the density of CNWs. An electric stimulation through the CNWs scaffold shows further interesting effects on culturing and differentiation of cells strongly depending on its frequency. These results suggest the interesting properties and diverse applicability of both CNWs and their composites.

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The properties (and some applications) of graphene grown at high T on Co

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Abstract:
Graphene grows onto cobalt by means of diffusion of carbon atoms during the isothermal stage of exposure to hydrocarbon precursor, followed by precipitation during cooling. This method, largely applied with nickel catalyst, is known to produce continuous, but not uniform, layers with the concurrent presence of mono- and poly-graphene areas. With the aid of Raman mapping of graphene still lying onto its catalyst, we are able to consider the possible origins for the observed distortions of the phonon modes with respect to the well-known picture of the monolayer material suggesting some observations to be interpreted in terms of the occurrence of isotropic strain with the uniaxial component superimposed at the metal discontinuities. The observation of strain in as-grown graphene opens the possibility of tailoring the electronic density of states via strain engineering directly during growth.
The material is not damaged by the laser during Raman investigation, differently to the Cu-grown material, whereas excess of precipitation has the beneficial effect to enhance its mechanical stability allowing for the easy transfer without the aid of any polymeric support. This makes our graphene particularly suited for the realization of suspended membranes. In the present presentation I will focus onto one possible application of such membranes that is the realization of suspended lithographic masks for shadow evaporation. This technique, which is largely used for realizing mesoscopic devices where the quality requirements for the junctions prevents the exposure to ambient air and the occurrence of quantum phenomena requires highly defined structures, can be improved by the use of pure 2-dimensional masks, like the graphene ones. Advantages and differences with respect to the polymers commonly employed, are presented and discussed.

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Electrochemical lithiation of epitaxial graphene for rechargeable batteries

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Abstract:

The development of next-generation energy storage devices possessing enhanced performance, especially lithium-ion batteries (LIBs) requires both incorporation of new LIB's components, namely electrodes to existing technologies and a deep understanding of the interfacial chemistry of electrode materials interacting with lithium species. Owing to its extraordinary chemical and thermal stability, large active surface area and wide potential window graphene-covered SiC has been proposed earlier as a promising anode material in LIBs [1, 2]. Having dangling-bond-free surface, high crystalline quality and exceptionally high electrical conductivity, graphene plays a pivotal role in improving the capacity of the SiC anode. Particularly, graphitization activates the inert SiC matrix, enabling high performance lithium insertion. Indeed, it was shown that growth of epitaxial graphene (EG) on doped 6H-SiC (0001) gives rise to enhancement of the Li-ion capacity to the value of 670 ± 130 mAh/g, which is much higher than the graphite capacity limit [1]. Further development of LIBs exploiting epitaxial graphene on SiC as an anode unambiguously demands achievement of more reliable control of the lithiation process. Here we apply the electrochemical intercalation approach to explore the electrochemical activity of Li on monolayer epitaxial graphene grown by thermal decomposition of the 4H-SiC substrate in argon atmosphere. Metallic lithium deposition (cathodic process) on the electrode occurs at a potential of around -3.482 V, while reverse reaction (anodic process) is observed at -3.009 V. Peak-to-peak separation was estimated to be ~ 473 mV, indicating that Li-related redox process at the surface of EG/4H-SiC is an electrochemically quasi-reversible process. Reduction current densities up to 1 $A \cdot dm^{-2}$ at a potential of ~-3.48 V were registered during cyclic voltammetry. Chronoamperometry measurements allowed us to gain insights into the Li electrochemistry at the graphene/buffer layer/Si-face 4H-SiC interface. By performing in-depth Raman mapping analysis, we shed light on the nature of the structural changes of the epitaxial graphene induced by electrochemical lithiation. Density functional theory calculations were used to study lithiation mechanisms of EG/4H-SiC.

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Growing Highly Pure Semiconducting Carbon Nanotubes for Nanoelectronics by Electrotwisting the Helicity

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Abstract:
Carbon nanotubes (CNTs) are anticipated to be the successor to silicon in next generation integrated circuits. However, great challenges to the practical application of this concept include the need to grow horizontal semiconducting CNT (s-CNT) arrays with very high purity. Recently, we found that charge is generated during the CVD growth of CNTs [1], which inspired us to use electric field to twists the helicity of the CNTs during synthesis. As a result, nearly-defect-free s-CNTs horizontally-aligned on the substrate have been synthesized with less than 0.1% residual metallic CNT (m-CNT), thus offers a potential pathway to practical applications of CNT nanoelectronics [2].

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Application of low-cost MWCNT/polymer based heating elements as room temperature NIR bolometers with high signal to noise ratio

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Abstract:
Multi-walled carbon nanotube networks have been demonstrated to enable the realization of flexible and low-cost electrical heaters, often combined with interesting sensing properties. In order to enhance the stability they are often embedded into a polymeric or epoxy matrix material, that on the other hand strongly modifies the actuating and sensing properties [1,2,3].
One of the most promising applications of nanotube networks in optoelectronic applications, besides their use as hetero-emitters and transparent conducting contacts in solar cells, is their application as sensitive bolometers without need of external cooling. While in the case of single-walled carbon nanotubes even wavelength selective bolometers can be realized [4], multi-walled carbon nanotube based bolometers have generally demonstrated a higher sensitivity and also a faster response [5].
A series of very common nanocomposite based electrical heaters have been investigated regarding their room-temperature bolometer functionality in the near-infrared wavelength range. In particular devices with syndiotactic polystyrene, high-density polyethylene and epoxy resin as matrix materials, all realized with the same type of MWCNT filler, have been investigated. First of all, we obtained - with the appropriate contact material - in all cases a perfectly linear current-voltage characteristics and very good room-temperature conductivity stability. In the case of the polystyrene based nanocomposite material, however, this had only be achieved after a prior Joule heating burn-in procedure. Using LEDs at 780nm and 1300nm for excitation we could for all three materials demonstrate linear, with respect to the light intensity, bolometer operation with good long-term stability and a very good signal-to-noise ratio.

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Elasto-mechanical study of MoS_2 domes by Atomic Force Microscopy and Spectroscopy

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Abstract:

The mechanical, electronic and optical properties of van der Waals Transition Metal Dichalcogenides offer exciting opportunities for the design of new materials and devices, by combining extremely high stiffness, bending flexibility and tunable electrical and optical properties. In particular, the possibility of controlling the spatial variations of such properties by micrometer and sub-micrometer patterning is considered to have a great impact both for applied and fundamental research.

Here, we study the morphological and elasto-mechanical properties of atomically thin MoS_2 membranes under tensile strain by using nano-indentation experiments based on atomic force microscopy and spectroscopy (AFM/AFS). The membranes were fabricated by exploiting the effects of H^+ irradiation on bulk MoS_2 flakes [1]. Therein, the formation and coalescence of molecular H_2 just one or few monolayers beneath the crystal basal plane leads to the creation of MoS_2 spherical membranes (or domes) filled with H_2 gas and protruding from the sample surface. The dome formation can be engineered by depositing -prior to H^+ irradiation- a hydrogen-opaque mask with circular openings of micrometer-scale radius. This results in both a precise control of dome's nucleation sites and fine tuning of their size. AFM analyses demonstrate that, despite the change in size of the openings, the ratio between height and radius of the domes, a quantity proportional to the local strain, keeps a constant value. In addition to this, AFS experiments allow us to quantify both the 2D Young's modulus of MoS_2 membrane, when strained in the shape of domes, and the 3D Young's modulus of MoS_2 flake. By interpreting our results in the framework of a membrane model [2], we quantify the pressure of H_2 and the number of gas particles inside the domes, along with an adhesion energy of 60÷150 meV/Å between the blistered membrane and the parent MoS_2 flake, as a function of the dome size. Finally, we show that the domes are very robust with respect to nano-indentations exerted by using external loads as high as 2.25 μN. Indeed, our experiments demonstrate that only 5% of more than one hundred sampled domes get damaged due to the high-load AFS solicitation.

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Analysis of zinc ions supersaturation during the growth of ZnO nanorods

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Abstract:
Zinc oxide is a wide band gap semiconductor with many potential applications in nanoscale devices in photonics and electronics. Particularly ZnO nanostructures have been widely studied in the last few decades. There are plenty of different methods to prepare zinc oxide nanorods either from gas phase or from liquid phase. Very frequently used method is chemical bath deposition (CBD), which belongs to the second group. CBD is commonly carried out in a regular batch reactor with a precursor solution in which the nanorods are grown on a seeded substrate at increased temperature. In our studies, we use as a precursor for ZnO synthesis a solution of equimolar amount of zinc nitrate and hexamethylenetetramine (HMTA). To obtain well-ordered nanorods with a high degree of reproducibility, it is necessary to control the growth conditions and to understand the growth mechanism that can change during the growth. The way to estimate the growth conditions, especially the varying concentration in solution, is a quantitative chemical analysis. Titration is a suitable non-expensive and reliable analysis in our chemical system. Titration is useful for the estimation of unknown molar mass of identified substance in an analyte solution. A chelatometric titration was used to determine the decrease of zinc ion concentration caused by consumption of the growth units during the precipitation of zinc oxide. The dependence of the zinc ion concentration on the growth time and temperature was measured. The obtained concentration profile provided information on the reaction kinetics. Moreover, together with the SEM image analysis of the grown nanorods, the zinc ion supersaturation was determined. The obtained data were then compared with modeled supersaturation data and the growth mechanism was deduced.

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Functionalization of carbon nanotubes for nitroaromatic explosive detection

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Abstract:

Carbon Nanotubes (CNT) are considered as promising materials for many type new electronic devices due to their unique electronic structure and electric properties. In particular CNTs with suitable functional groups bonded to CNT surface can be used to reveal different chemical compounds.

CNT based chemiresistors show promising performances in explosive sensing [Schnorr et al]. CNT chemiresistors can be deposited between electrodes by evaporation or dispersions, or can be effectively drawn from compressed CNT solids.

Both these systems demonstrated a very high sensitivity in detecting explosives, in particular molecules of trinitrotoluene (TNT), which is a common explosive used in improvised explosive devices (IED). Moreover in such nanostructures the signal detection is based on conductance changes of the nanostructures in air, with cycles of detection and sensor recovery that can be performed by simple systems and with very low electrical power requirement.

In the present work we present the synthesis and functionalization of CNTs with amino groups to prepare sensors for detecting explosives, in particular nitroaromatic explosives such as TNT. Multiwalled carbon nanotubes are used for the realization of devices with improved detection limit and selectivity to different types of notroaromatic explosives.

Two type of CNTs (in powder form or by direct deposition on the silicon substrates) have been grown by aerosol-chemical vapor deposition (A-CVD) technique from SCIDRE (Germany) and analyzed by X-Ray diffraction, SEM, TEM and Raman spectroscopy. Very smooth and long CNTs with good electrical conductive properties are obtained.

Three step of functionalization process have been performed: Oxidation (carboxylation-COOH), amidation and amino functionalization.

For amidation we used the relatively simple gas phase amidation method, treating carboxylated CNTs with ammonia gas at high (~250^{0}C) temperatures

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Posters

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P01

Optimized Model for Non-ideal Organic Electrochemical Transistors Impedance

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Abstract:
Organic electrochemical transistors (OECTs) offer a powerful functionality for both sensing and neuro-inspired electronics [1] with still much to understand on their time-dependent behavior. OECTs based on PEDOT:PSS conducting polymer have revealed two distinctive operation regimes of a device: a low frequency and a higher frequency regimes dominated by the conductance of the polymer and of the gating electrolyte, respectively [2]. However, the systematically observed non-idealities in the impedance spectra over the large frequency range and ionic concentrations caused by both the materials and the device complexity cannot be explained by simple models.
We report on modeling of OECTs by an optimized equivalent circuit model that takes into account the frequency dependence of the device impedance from 1 Hz to 1 MHz for a large ionic concentration range (10^{-4} – 1 M) and various chemical nature of the ions.
Based on experimental data for $KCl_{(aq)}$ and $CaCl_{2(aq)}$. the model explains the time dependency of the OECT as a whole and discusses the sensibility of new introduced elements pseudo-capacitance and inductance to concentration and voltage to understand the local physics. In particular, the observed concentration-dependent negative phase change in the impedance suggests an inductive contribution to the device impedance due to the doping/dedoping process in the organic layer driven by the applied harmonic voltage as an underlying mechanism. The introduction of these non-redundant elements and the study of their behaviors as function of ionic concentration and applied voltage give a more detailed picture of the OECT working principles at a specific time domains which are highly relevant for multi-parametric ion sensing and neuromorphic computing.

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P02

Optical Effects produced by Cadmium insertion in ZnO

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Abstract:
The ZnO is a member of the broad family of II-VI semiconductor. In addition to its broad bandgap, the high bonding energy of excitons ensures an additional emission source, increasing the possibilities of optoelectronic applications. The controlled insertion of transition metals in ZnO offers the possibility to tailor the levels in the visible range associated with point deffects. We present here a study of the influence of cadmium insertion in the structural and optical properties of ZnO.. Among the objectives to be achieved, stands out the understanding and the mastering in the production of this compound through the tuning of the synthesis parameters. Samples of $Zn_{1-x}Cd_xO$, with x=0.0 and x=0.01 were produced by mechanical alloying using thermal treatments at 200°C, 400°C and 700°C, in order to induce changes in crystallinity, internal stress relaxation and homogenization of the composition. The influence of the synthesis parameters was investigated using X-ray diffraction, Raman spectroscopy and photoluminescence. Special attention is given to the interplay between the morphological (surface area) and structural (points defects) characteristics and the resulting photoluminescence. Through the XRD data was identified the presence of wurtzite phase for all samples, without any other phase, as well as that the insertion of Cd and processing temperatures do not interfere in the long-range order. The Raman analysis has proven to be sensitive to the insertion of Cd even in extremely low concentration, evidenced by the activation of the modes prohibited by selection rules and intensification in the localization of the phonons. The IR-visible photoluminesce is formed by the spectral contribution of five different transitions. The temperature of treatment is a fundamental parameter for luminesce efficiency. For higher temperatures the photoluminescence undergoes a strong suppression. Through temperature dependent photoluminescence we show that the strong red shift in the maximum of the emission caused by the Cd insertion is due to the increase in the emission intensity associated with excess oxygen, which is corroborated by Raman analyses.

P03

Optimization of wear resistance of knee joint implant made of titanium alloy with coating treatments and UHMWPE reinforced by carbon nano-filler and cryogenic treatment using Taguchi method

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Abstract:
Knee Joint Implant is mostly made of Titanium-alloy femoral and UHMWPE tibias. Wear and friction are the main problems of knee joint implant. Surface treatments, such as cryogenic and coating, and Nano-particle reinforcement influence friction and wear of contacting parts. The paper aims to investigate the effect of cryogenic process parameters, coating materials, lubricant and % of reinforced carbon Nano-filler on friction and wear of knee joints. The experimental testing and Taguchi method has been applied to investigate the effect of the mentioned parameters in order to achieved the lowest friction and wear of the knee joint components with minimum number of experiments. The wear experiments were carried out on a ball-on-disc testing machine according to G99 standard under dry condition. In this study, three parameters at three levels were study using Taguchi L9 array table. Titanium Alloy were treated with Cryogenic process at three different rates and then coated with DLC and TiN and one uncoated. UHMWPE were reinforced with three different % of carbon Nano-filler using extrusion process. Two experiments were carried out using the same testing conditions. Hardness and surface roughness testing and morphological observations were performed on specimens before and after the wear testing experiments. Friction coefficient and wear volume of were measured. Using the Friction coefficient and wear volume results, Taguchi main effect S/N response and plot were calculated for each output. Taguchi main effect analysis and ANOVA results show that the coating is the most important factors influencing the friction coefficient. The % of reinforced particle is the most important factors influencing the wear volume of UHMWPE. The cryogenic parameter is the most important factors influencing the wear volume of Titanium Alloy. Applying the Taguchi method and using the minimum wear volume for both Titanium Alloy and UHMWPE as the design criterion, the optimum process design was identified. The Taguchi predicted response was confirmed by the experimental test. The main factors effecting friction and wear were studied. The optimum treatment condition and % of nano-fiber reinforcement, which will reduce friction and wear of both femoral and tibias knee implant components, were
identified. The Taguchi predicted response was confirmed by the experimental test.

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P04

Nanostructured electrochemical platform used for gluten presence evaluation

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Abstract:
Different nanostructures are used for food alergen detection and food safty [1, 2]. They can offer methods that are reliable, accurate, and highly sensitive. Amoung these nanostructures we can mention: metal oxides (titanium, gold or silver oxides) and nanotubes (carbon and graphene) [1].

In this research area, different types of nanosensors where used. These include: electrochemical, optical, quartz crystal microbalance (QCM), cantilever or magnetic sensors Electrochemical sensors are based on: electrical current, potential, conductance, or impedance measurements at the electrode / sample matrix interface. Advantages of electrochemical sensors are: sensitivity, good performance with colored and turbid samples, simplicity, speed, and compatibility with portable measurement devices [2].

The present study, present research in food alergen detection using electrochemical detection via nanostructures. Electroochemical detection method used in this study was differential pulse voltammetry. As a nanostructured platform we used titanium dioxide nanostructures modified with graphene oxide. Two type of TiO_2 nanostructures where prepared: nanotubes and nanofibers. Nanotubes where obtained by electrochemical anodization. Naofibers where obtained by electrospining. After nanostructures optimization, graphene oxide deposition was performed usig three different methods. Cyclic voltammetry was the method that led to the best results. In the end, different electrochemical tests where performed for gluten presence evaluation. Modified nanostrucutred electrode was used as working electrode for gluten presence determination from known concentration gluten solutions and food samples.

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P05

Sensors based on carbon nanotubes and germanium nanowires for explosive detection

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Abstract:

TNT belongs to the class of nitroaromatic explosives which represent large part of the most common explosives. Semiconducting nanowires can detect TNT down to a detection limit of ~1x10^{-6} ppt by proper surface functionalization with an electron-rich amino-silane which binds the explosive molecules of TNT through charge-transfer donor-acceptor interactions causing sharp changes in the conductance of MW [1]. Carbon nanotubes (CNT) are highly responsive to their physical and chemical environment. CNT are unique among nanoscale sensor platforms in their ability to detect the adsorption of as few as a single molecule of an analyte [2]. CNT based chemiresistors display promising performance in explosive sensing. The hot wall vapour phase epitaxy using iso-butil-germane and gold nanoparticle colloids was used to grow Ge NWs. First attempts to functionalize the NWs surface have been performed by long chain alkanethiols terminating with an amino group. The electron-rich amino groups provide the passivation of the NWs surface and bind the electron-deficient explosive molecules of TNT through charge-transfer donor-acceptor interactions, affecting the conductance of the NWs. Single NWs were contacted to Au electrodes with Pt deposited by focused ion beam. I-V characteristics showed the ohmic nature of Pt-NW contacts and electrical resistivity values in the 0.05 - 0.5 ohm cm range. Aerosol-assisted CVD and arc-discharge methods have been used for synthesizing single wall carbon nanotubes. Cyclohexane and hexane, metallocenes have been used as carbon sources and catalyst, respectively. For the functionalization of CNTs with amino groups different approaches have been followed:

- Preliminary oxidation of the CNT surface by treatment with H_2SO_4/HNO_3 to generate carboxylic acid moieties that are subsequently exploited to anchor the sensing group through the formation of ester or amide bonds.
- "Prato reaction" [3] as a method of functionalization of nanostructures alternative to the above described sequence oxidation-condensation sequence.

First characterizations of the successful functionalization of nanostructures are reported.

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P06

Influence of citric acid and oleic acid coating on the dc magnetic properties of Fe_3O_4 magnetic nanoparticles

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Abstract:

The properties of two samples of Fe3O4 magnetic nanoparticles coated with citric acid and oleic acid respectively, have been analysed by means of DC magnetic measurements. The analysis has been performed by measuring the Zero Field Cooling (ZFC) and Field Cooling (FC) curves of the samples at different applied fields. In this framework, the blocking temperature distribution, the clusters behaviour and the effect of the coatings on the experimentally evaluated samples properties have been discussed. Moreover, after the evaluation of the blocking temperature T_B, the magnetization as a function of the field, M(H), has been measured above and below T_B and the comparison between the results for the two samples has been discussed.

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P07

Field Emission Characterization of MoS_2 Nanoflowers

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Abstract:
Nanostructured materials have wide potential applicability as field emitters due to their high aspect ratio. We hydrothermally synthesized MoS_2 nanoflowers on copper foil and characterized their field emission properties, by applying a tip-anode configuration in which a tungsten tip with curvature radius down to 30–100 nm has been used as the anode to measure local properties from small areas down to 1–100 μm^2. We demonstrate that MoS_2 nanoflowers can be competitive with other well-established field emitters. Indeed, we show that a stable field emission current can be measured with a turn-on field as low as 12 V/μm and a field enhancement factor up to 880 at 0.6 μm cathode–anode separation distance [1].

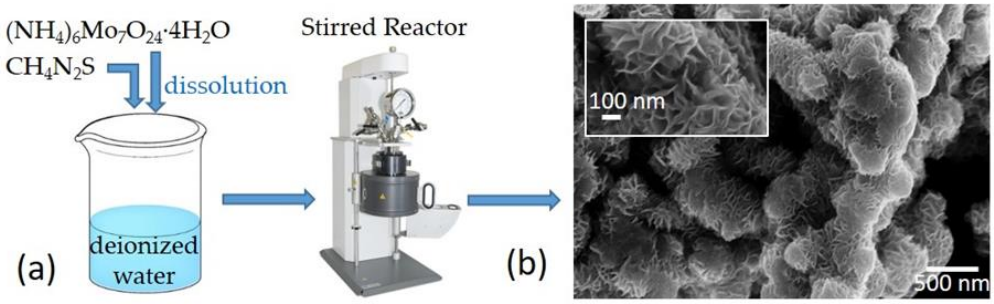

Figure 1. (a) Schematic of the MoS_2 synthesis by the hydrothermal method; (b) Scanning electron microscope image of a MoS_2 nanoflower.

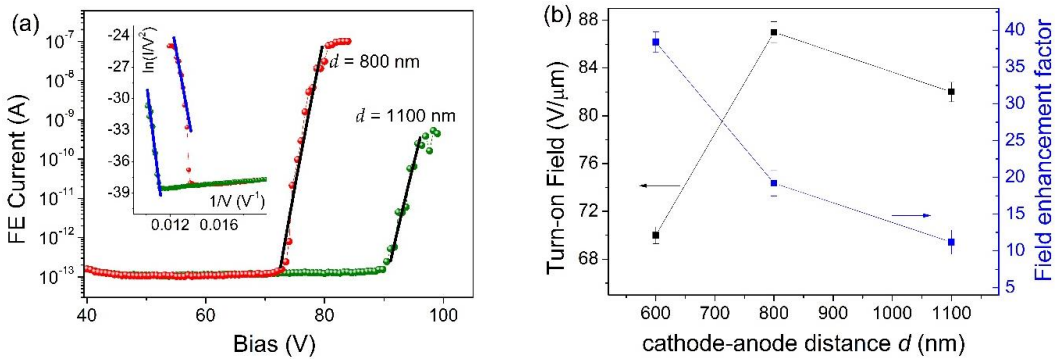

Figure 2. Effect of cathode–anode separation distance variation on the FE I–V characteristics. (a) Curves are measured for d = 800 nm and 1100 nm and are compared to theoretical FN behavior (solid lines). Inset: FN-plots and linear fittings. (b) Dependence of the turn-on field and of the field enhancement factor on the cathode–anode separation distance d.

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P08

Effect of different atmosphere on the synthesis of $Ba_2CuGe_2O_7$ single crystals

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Abstract:

A ferroic compound is a material which exhibits a hysteresis cycle of a specific physical property when subjected to an external cyclic stimulus, that can be electric, magnetic or mechanical. For example, a ferroelectric material can acquire a spontaneous electrical polarization that can be reversed by the application of an external electric field. However, the polarization depends not only on the electric field, but also the electric field history. Those materials which simultaneously show two or more different ferroic orders are called multiferroic and, among them, systems that are instantaneously ferroelectric and ferromagnetic are extremely important and useful for many technological applications. Unfortunately, they are not very common and, indeed, generally ferroelectricity and magnetism are coupled by weak interactions only. For this reason, the research in this field is looking for innovative materials with large coupling.

Among them, such properties are observed in $Ba_2CuGe_2O_7$, that is, indeed, a system particularly intriguing because of its complex magnetic phase diagram. $Ba_2CuGe_2O_7$ crystallizes in the space group $P\bar{4}2_1m$ with a non centrosymmetric tetragonal structure. The lattice parameters are $a = b =$ 8.466 Å and c = 5.455 Å.

Details on the growth of large, defect-free $Ba_2CuGe_2O_7$ crystals by the floating zone method employing two different routes are reported. This method is generally considered a powerful tool for the growth of high purity single crystals of a very large class of materials, including many complex oxides. The quality of the crystals depends on many experimental parameters, such the temperature and the thermal gradient, the translation rate, and the composition. The nature of atmosphere (i.e. its composition and pressure), in which the crystal growth process is performed, also plays an important role. For many different systems, even slight modifications to the growth atmosphere can lead to drastic changes in the physical properties of the samples that are grown.

Morphological, compositional and magnetic properties of single crystals of $Ba_2CuGe_2O_7$ grown in oxygen and in dry air have been investigated. It is shown that the use of different atmospheres influences the morphological and compositional characteristics, probably because of some secondary reactions, that occur on the surface of the sample when oxygen is used, but it does not change the structural and magnetic properties. In the case of samples grown in oxygen, a thin, dark superficial layer forms. In this layer impurity particles of $BaCu_2Ge_2O_7$ are present, while the core is formed by pure $Ba_2CuGe_2O_7$.

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P09

Field-emission properties of β-Ga_2O_3 nanopillars

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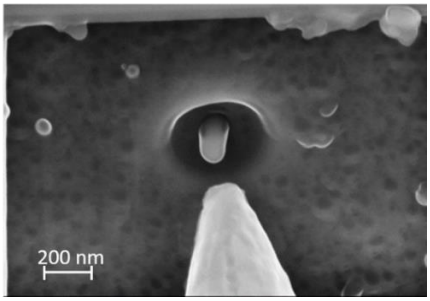
Abstract:
Gallium Oxide (Ga_2O_3) is considered a promising candidate for high power electronics application because of its excellent physical and chemical properties[1]. Among the five polymorphs, the β-Ga_2O_3 is the thermodynamically most stable. It has a wide bandgap of about 4.8 eV and a very high breakdown electric field (E_{br} ~ 8 $MVcm^{-1}$), three times larger than that of SiC and GaN, which enable handling huge switching voltages. Moreover, the Baliga figure of merit (BFOM=$\varepsilon\mu E_g$, where ε is the relative dielectric constant, μ is the electron mobility and E_g is the bandgap of the semiconductor), a parameter used to assess the suitability of a semiconductor for power device applications, is several times higher than that of SiC and GaN. Hence, β-Ga_2O_3 based power devices offer a significant reduction of the current loss. Despite the recent interest in this material, few research groups have explored opportunities for different applications, such as field emission. We focus on the field emission from gallium-oxide (β-Ga_2O_3) nanopillars, etched by Ne^+ ion milling on β-polymorph (100) single crystals. A stable field emission current, with a record density over 90 A/cm^2 and a turn on field of ~30 V/μm, is achieved[2,3]. The high field enhancement factor of about 200 at 1 μm cathode-anode distance can be further increased by optimizing the shape of the nanopillar apex. This work demonstrates that the material properties combined with an appropriate nano-patterning can make β-Ga_2O_3 competitive or better than other well-established field emitters.



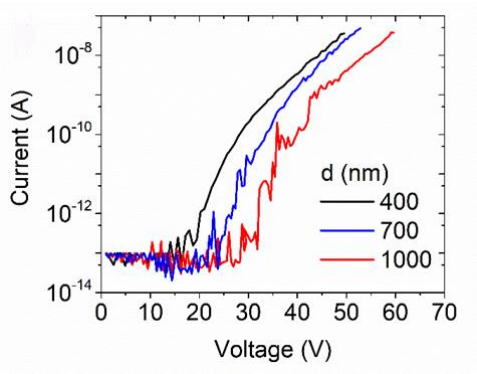


Fig 1 – SEM image of the β-Ga_2O_3 single nanopillar and field emission characteristic at different distances between the tip and the pillar

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P10

Magnetic monodispersed nanoparticles as drug carriers: a simulation and experimental study of Fe_3O_4 and temozolomide with nanometer precision size control.

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Abstract:
Chemotherapeutic advancements in recent years have provided increased hope to people diagnosed with many different types of extracranial cancers. The interaction with the blood-brain barrier (BBB) remains a major challenge in effective chemotherapy of brain metastases. Despite the variability in its barrier function within brain tumor lesions, most drugs are still prevented from effectively entering the brain. The chemotherapy drug, temozolomide (TMZ) is no exception and it has been shown that its concentration in the cerebrospinal fluid is only 20% of that measured in the plasma of patients. As such, it is clear that improved delivery methods of this chemotherapy drug remain a priority in research and development.

It is well known that iron oxide nanoparticles (NP), in specific magnetite with a Fe_3O_4 stoichiometry, are non-toxic, bio-degradable, inexpensive, relatively easy to be tuned and functionalized for targeted applications as well as biocompatible. Its superparamagnetic properties also make these NPs ideal for targeted delivery vehicles *via* external magnetic fields and for contrast enhancement in magnetic resonant imaging (MRI).

Despite great progress in the synthesis of iron-oxide NPs using thermal decomposition methods, production of NPs with a low polydispersity index is still a challenge. To narrow down the size distribution, size selective precipitation processes have to be performed. In this study we show that, for the first time, the production of monodisperse iron-oxide NPs are indeed possible without employing any post synthesis size-selective procedures. The study shows that at a very specific acid/amine ratio, different synthesis procedures may yield truly monodisperse NPs with polydispersity of less than 7%. We were able to predict this specific ratio by performing molecular dynamic simulations in advance that revealed a maximization of binding energy at this ratio.

We further report on the interaction of TMZ with Fe_3O_4 NPs with particular reference to the different bonding modes: chemisorption, physisorption and hydrogen bonding as a function of NP size and TMZ loading (dose). This is done to investigate not only effective drug delivery, but also to address leakage of the drug molecules before reaching the target.

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P11

The determination of polycyclic aromatic hydrocarbons content in exhaust gases formed during carbon nanomaterials synthesis

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Abstract:
Carbon nanomaterials are commonly used in various branches of science, technology and industry. It is known that during the process of carbon nanomaterials synthesis gaseous products and various unknown toxic hydrocarbons are formed. Detailed analysis of all gaseous products during pyrolysis process is needed in order to clarify the nature of the formed substances and to control the technological characteristics of the catalyst. The chemical composition study of exhaust gases on the facility of propane-butane mixture pyrolysis for carbon nanomaterials synthesis was made. The 16 polycyclic aromatic hydrocarbons (PAHs) analysis of the extracts from exhaust gases was carried out by a gas chromatography-mass spectrometry method ISO 11338-1:2003. It was established that the concentrations of some PAHs exceed as 14, 20, 90 and 100 times much as the maximum permissible concentration in the air. Thus, the production of carbon nanomaterials could damage the environment. It was found out that appropriate devices should be used during the production of carbon nanomaterials in order to eliminate the PAHs that proceeding into environment. The data obtained allows to assess the degree of danger to the environment and the possible contribution of such facilities to environmental pollution, as well as to use protective instruments to reduce harmful effects.

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P12

Effect of electron irradiation and field emission from MoS_2

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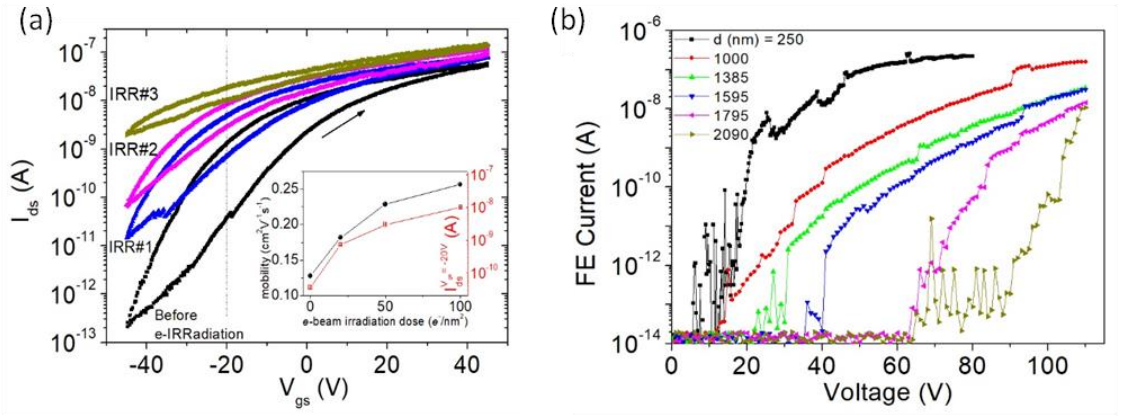
Abstract:

During the last few years an increasing interest in 2D materials for technological applications is erasing. Anyway, the development of TMDs-based nanoelectronics needs to overcome the difficulties related to point defects as well as structural damages and dislocations, often generated during the fabrication processes and characterization activities. For instance, the exposure to electrons or ions bombardment can provoke relevant modifications of the structure introducing damage and/or defects, involving a dramatically change of the electrical properties. In order to understand what problems are related to the electron beam (e-beam) exposure, we perform a systematic electrical characterization of CVD synthesized few-layer MoS_2 based FETs, inside a scanning electron microscope. We study the effects of low energy (up to 10 keV) e-beam irradiation reporting an increase of the carrier mobility and a negative shift of the threshold voltage for successive low energy irradiations that is explained in terms of positive charge trapped in the SiO_2 gate dielectric [1]. We also perform a complete characterization of the field emission properties of the few-layer MoS_2, that due to the intrinsically sharp edges and high aspect ratio is a natural candidate to realize high performance field emission cathodes [2]. We observe that, for small cathode-anode distances to $d \approx 1.5\mu$m, the field enhancement factor increases with the distance; vice versa, for cathode-anode separation greater than 1.5 μm, we clearly observe that field enhancement factor is rapidly decreasing for increasing distance. We demonstrate low turn-on field and quite high field enhancement factor, at anode-cathode distance of the order of few μm, showing that MoS_2 allows high current emission with high time stability, with fluctuations of the order of 5%.



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P13

Ag/GO Nanocatalysts for N-Alkylation

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Abstract:
The development of C-N bond is of great importance in synthetic organic chemistry because the nitrogen-containing compounds especially amines are the key intermediates in agrochemicals, bioactive molecules, pharmaceuticals and natural products. N-alkylated amines are usually prepared via the reaction of amines with alkyl halides, reductive amination with carbonyl compounds and hydroaminations or hydroaminomethylations. But these methods have some serious drawbacks; e.g., toxic nature of the reagents, generation of many by-products and over alkylation. Recently, hydrogen or hydrogen auto transfer methodology, has become a useful way to obtain amine derivatives, where water is the only side product. For this process many homogeneous transition metal catalysts, such as ruthenium, platinum, iridium, silver, palladium and some heterogeneous catalysts, such as Pd/MgO, Ag/Mo, Au/TiO_2, Cu/Ni-based and Fe_3O_4 have been used. On the other hand, many of these methods suffer from harsh reaction conditions, toxic and capricious ligands, and high catalyst loading. Among these Ag NPs attracted special attention due to their interesting nanostructure and catalytic properties. Therefore, environment-friendly catalytic process is very demanding for the N-alkylation of amines with alcohols.
To minimize the catalyst loading in the reaction the catalytic site should be highly dispersed over a high surface area matrix. For this reason graphene, a promising carbon material, has excellent mechanical properties, a large surface area, and a distinctive two-dimensional structure, providing an ideal platform to anchor functional groups and embed nanoparticles. In particular graphene oxide (GO) contains a range of reactive oxygen surface functional groups, can be easily modified and dispersed in water, and used as support for nanoparticles dispersion and stabilization, moreover, graphene oxide is a good mediating agent for site-selective allylation of functionalized thiophenes with readily accessible alcohols. Furthermore, due to its moderate Brønsted acidity, activity surface moieties, and possible implementation into composite materials, GO has already found elegant applications in several synthetic organic.
Here we report, for the first time, the catalytic activity towards N-alkylation reactions of Ag/GO nanocatalysts. Ag/GO nanocatalyst was obtained through a “green” approach and directly used in N-alkylation of aniline, showing high conversion and selectivity in short times and mild conditions.

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P14

OPTICAL GRADE EPOXY-METAL NANOCOMPOSITES AS ENCAPSULATING FOR DIFFUSE LIGHT-EMITTING DIODES

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Abstract:
Optical grade epoxy resins are used for the encapsulation of light-emitting diodes (LEDs). Usually LEDs are used as collimated light sources (actually, cone-shaped light is emitted), however there are many technological applications that may benefit of LEDs able to produce diffuse light. The cone-shaped light, generated by the LED reflective cavity, can be converted to diffuse light by dispersing nanoparticles of a convenient size in the epoxy case. In fact, nanoparticles interact with collimated light, producing a scattering phenomenon (Faraday-Tyndal effect). Since nanoparticles are commonly generated by wet synthesis techniques, their transferring to the epoxy resin without aggregation is not an easy process. Here, a new method for the *in situ* generation of metal nanoparticles in epoxy resins has been developed. This method is based on the thermolysis of non-polar organic salts (e.g., AuCl to generate gold nanoparticles, (1,5-cyclooctadiene) (hexafluoro-acetylacetonate) silver(I), [Ag(hfac)(COD)], to generate silver nanoparticles, etc.) dissolved in the epoxy. Thermolysis was induced by heating the epoxy-metal precursor solution in a microwave oven before hardener addition. The epoxy-metal nanocomposite samples were cured in air at room temperature, and were characterized by transmission electron microscopy (TEM) and optical spectroscopy (UV-Vis), to establish the nanocomposite morphology (nanoparticle average size, presence of aggregates, etc.) and optical properties, respectively. Depending of metal precursor type, two different morphologies were achieved: (i) contact-free dispersion of spherical and quite monodispersed nanoparticles, and (ii) aggregated shape-less nanoparticles. In particular, the thermolysis reaction of the metal precursor generates both a metallic atom and a molecular fragment. Such molecular fragment may have a more or less pronounced surface stabilizing effect. The thermal decomposition of AuCl produced chlorine atoms that are not able to protect the electrophilic gold nanoparticle surface during their growth, and consequently the achieved nanoparticles were shape-less and formed small aggregates (see Figure 1a). Differently, the thermal decomposition of [Ag(hfac)(COD)] generates an organic fragment (hexafluoro-acetylacetonate), which is able to protect efficiently the silver nanoparticle surface from aggregation (see Figure 1b). Figure 1c shows how efficiently the epoxy-Ag nanocomposite is able to scatter the light emitted by a red LED.

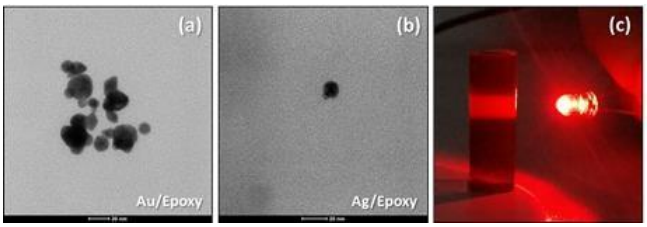

Fig. 1 – TEM micrograph of: epoxy-Au nanocomposite (a), epoxy-Ag nanocomposite (b), and image of the light scattering phenomenon in the epoxy-Ag nanocomposite (c).

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P15

The role of the substrate in graphene/Silicon Schottky diode

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Abstract:
The graphene/semiconductor junction is receiving increasing attention by scientists and engineers for its interesting basic physical properties and for the many potential applications. Graphene/semiconductor planar junction have been proposed as photodetectors, solar cells, chemical and biological sensors, rectifiers, etc. [1] These junctions have the potential to eliminate the need for p-n junctions with reduced depth in modern CMOS technologies and are, therefore, of considerable interest to the semiconductor industry. We have designed, fabricated and studied two different kind of graphene/silicon devices. The first device is obtained transferring CVD-synthesized graphene on a substrate of high doped n-Si patterned to form two-dimensional superficial arrays of nanometer-sized tips [2]. Graphene is laid on these tips forming Schottky nano-junctions. The device behaves as Schottky diode with a rectification factor increasing with decreasing temperature and greater than 100 at room temperature. The ideality factor of this diode tends to the unit value as the temperature increases. We observed almost linear increase in the height of the Schottky barrier moving from reverse to forward voltages, with a value of 0.36 ± 0.02 eV at zero bias. The original geometry of our device favours the absorption of light by multiple reflection on the silicon tips. Furthermore, the amplification of the electric field on the apex of the tips improves the separation of photogenerated charges and provides sufficient energy to start avalanche multiplication to impact ionization. This implies an increase of up to two orders of magnitude of the integral photoresponse ($3A/Wat\ 3mW/cm^2$ of intensity) in comparison to planar junctions. The second device was fabricated by transferring CVD-synthesized graphene on low doped n-type substrate [3,4]. The device achieves photoresponse as high as $3AW^{-1}$ and normalized detectivity > $3.5\times10^{12}cmHz^{1/2}W^{-1}$ in the visible range. The device exhibits a photocurrent exceeding the forward current, as photo-generated minority carriers, accumulated at Si/SiO_2 interface of the $Gr/SiO_2/Si$ capacitor, diffuse to the Gr/Si junction. We show that the same mechanism, when due to thermally generated carriers causes the increased leakage often measured in Gr/Si heterojunctions. At room temperature, we measure a zero-bias Schottky barrier height of 0.52eV, as well as an effective Richardson constant $A^{**}= 4\times10^{-5}$ Acm^{-2} K^{-2} and an ideality factor n ≈ 3.6, explained by a thin (<1 nm) oxide layer at the Gr/Si interface. Our devices are consequently a considerable contribution towards the development of graphene/silicon heterojunctions for optoelectronic applications.

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P16

SPICE Model for the Conduction Characteristics of Hexagonal Boron Nitride-Based Resistive Switching Devices

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Abstract
Equivalent circuit models are fundamental tools for incorporating resistive switching (RS) devices in complex architectures such as memory arrays and neuromorphic networks [1]. This does not strictly require a physics-based approach but the ability to deal with arbitrary input signals in standard electrical simulation environments like SPICE (Simulation Program with Integrated Circuit Emphasis). In this work, we apply a recently developed model to the simulation of the switching *I-V* characteristics of a 2D material such as hexagonal boron nitride (*h*BN) [2]. Devices with metal and multi-layer graphene (MLG) electrodes were investigated (Ti/MLG/*h*BN/MLG/Au and Ti/*h*BN/Cu [3]). The model follows a memristive approach [4], *i.e.* one equation for the electron transport and one equation for the memory state (hysteron) of the device. The devices were voltage ramped with positive and negative biases using a current compliance (CC) of 10 mA for the SET process. In this abstract, only the median *I-V* curves corresponding to 100 cycles are shown. Figure 1 corresponds to the *I-V* curve for Ti/*h*BN/Cu devices (red line). The model (blue line) is able to reconstruct the experimental data beyond the compliance limit. The green line is the hysteron. Figure 2 shows simulation results for a progressive reset. Intermediate memory states are perfectly achievable by the proposed model. Figure 3 shows the *I-V* curve for Ti/MLG/*h*BN/MLG/Au devices. The proposed model not only allows to reconstruct the whole *I-V* curve but can also deal with the high asymmetry between SET and RESET.

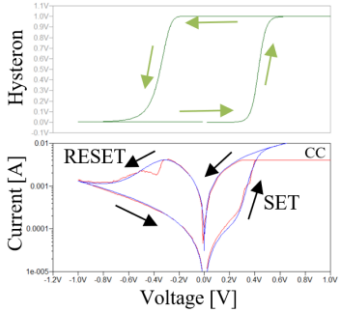

Fig. 1- Hysteron and I-V curves for Ti/hBN/Cu.

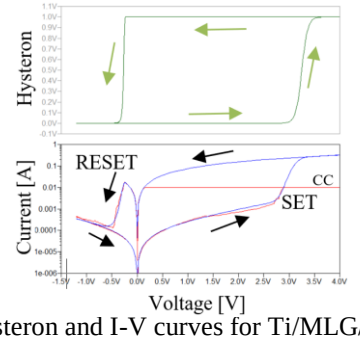

Fig. 3- Hysteron and I-V curves for Ti/MLG/hBN/MLG/Au.

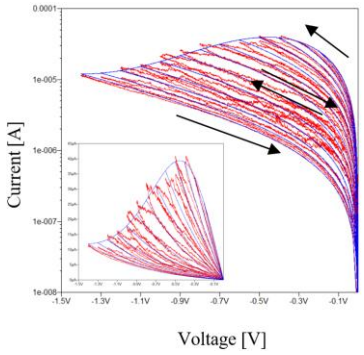

Fig. 2- I-V in linear and log axis for Ti/hBN/Cu device under progressive reset. Voltage and current as a function of time.

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P17

Nanoscale surface texturing of porous silicon carbide slabs by fs laser and plasma treatments

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Abstract:
Silicon carbide (SiC) has emerged as an outstanding material, which has proved to overcome the limitations of silicon in a variety of applications where robustness within prohibitive environments is required, such as in high-power electronics and in high-temperature energy conversion devices. In particular, SiC is the material of choice for solar radiation absorbers used in concentrated solar power (CSP) systems. One of the key issues to increase the efficiency of CSP systems is to decrease the emissivity of the absorbers. One possibility is to induce a proper surface patterning to tailor the optical properties of such absorbers elements. For this purpose, in this work two diverse approaches for inducing nanometer-scale surface-modifications of porous SiC slabs are investigated.
SiC slabs with 43% porosity were subjected to either femtosecond laser treatment or fluorine based reactive ion etching. We demonstrated that both techniques are capable of inducing significant and controllable surface morphology modification (Fig. 1) by the formation of needle like structures and ripples. These roughening features are found to be tunable by acting on the main process parameters, such as the translation speed and pulse repetition rate for the laser treatment, and RF-power, gas pressure and mixture for the reactive ion etching.

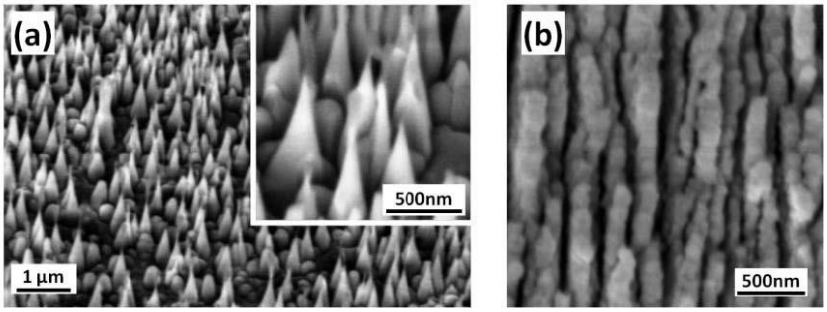

Fig1: SEM micrograph of SiC surfaces treated using a) fluorine based reactive ion etching and b) femtosecond laser, respectively.

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P18

Synthesis of Pt based dichalcogenides via thermally assisted conversion

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Abstract:
Group 10 2D layered materials present an interesting opportunity, due to the low temperature synthesis of such semiconductors within the thermal budget of back-end-of-line (BEOL) processing. Our experiments demonstrate thermally assisted conversion (TAC) of Pt in a scalable and controllable manner, into PtS_2 and $PtSe_2$. With synthesis temperatures in the order of 400°C, notably lower than typically associated with group-6 transition metal dichalcogenides (TMD), these materials have recently received considerable attention due to high carrier mobility and layer-dependent band gap. These materials demonstrate potential in high performance nanoelectronics, broadband optoelectronics and ultra-sensitive gas sensing. We examine numerous growth parameters, such as thickness, how the conversion pressure and sulfur abundance influences the stoichiometry of PtS_2, where sulfurization of Pt can result in both PtS and PtS_2 phases, and explore the impact the substrate has on the nature of the converted films.

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Crystallization in Vacuum-Deposited CuI/Cl_6Subpc bilayers for Photovoltaic Applications

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Abstract:
Today, subphthalocyanines are the most promising low-molecular-weight semiconductors for the thin-film photovoltaic cells employing fully organic planar- or multijunctions. Peripheral halogen substitution is known to increase the acceptor properties of a molecule and finally to result in *n*-type conductivity of thin films. However, the amorphous structure of thin vacuum-deposited films dominates the morphology and thus the transport of charge carriers. Structural templating offers an approach through which the morphology of phthalocyanine films can be modified [1].
In this work, we use the copper iodide (CuI) and elevated substrate temperatures to influence the growth of a hexachorinated subphthalocyanine derivative, Cl_6Subpc. The combination of these two materials in a bilayer is based on our previous experience in fabricating a hybrid planar heterojunction C_{60}/CuI, which contributes to the high photoconversion parameters of the semitranparent thin-film solar cells [2]. Therefore, CuI here plays the role of not only growth underlayer, but also the active *p*-type component of a photovoltaic junction.
Using X-ray diffraction, optical and atomic force microscopy, we traced the changes in the surface relief and structure of Cl_6Subpc films thermally deposited in vacuum on various functional substrates, including CuI. It was shown that the crystallization of the molecular layer can be controlled by varying the substrate material and temperature. This largely affects the Q-band splitting the optical spectra and the film conductivity.
Finally, the large improvement of the photovoltaic output in the model solar cells incorporating CuI/Cl_6Subpc was observed comparing to the reference samples with the non-structured bilayers. The results are potentially interesting for developing efficient nanodevices with a hybrid 'organic/inorganic' interface for the energy conversion.

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P20

Graphene nanoplatelets supported by low density polyethylene

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Abstract:

An advantageous micromechanical technique to deposit large area graphene nanoplatelet (GNP) thin films on a low-density polyethylene substrate is proposed. This method, based on the application of shear-stress and friction forces to a graphite platelets/ethanol paste on the surface of a polymeric substrate, allows to obtain films of overlapped nanoplatelets mainly made of 13-30 graphene layers as in the transmission electron microscopy (TEM) image shown below. The other measurements such as X-ray diffraction (XRD) and atomic force (AFM) support the occurrence of a partial exfoliation of the graphite platelets due to shear-stress and friction forces applied during film formation. Scanning electron microscopy (SEM) observations point out that the surface of the polymer is uniformly coated by GNP unities, and the TEM analysis reveals the tendency of the nanoplatelets to align parallel to the interfacial plane. It has been found that the deposited samples increases the resistance with increasing the temperature in the 15-40 °C range both in air and under vacuum. These structural and electrical characteristics will be compared to those of GNP films deposited by spraying a commercial graphite-based product on LDPE and glass substrates.

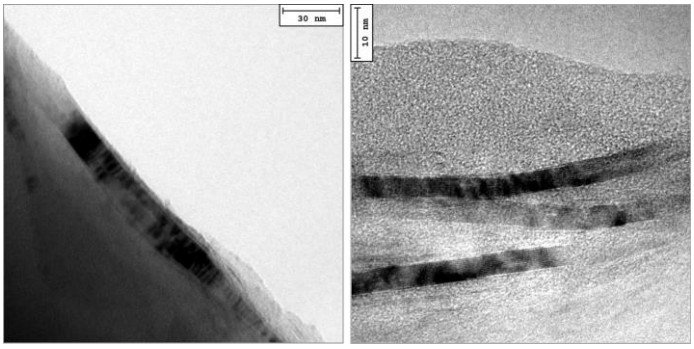

Fig. 1 – Cross sectional TEM micrographs of the GNP-LDPE sample.

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P21

Zn nanoparticle formation in FIB irradiated single crystal ZnO

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Abstract:
Zinc oxide (ZnO) is an outstanding material allowing for applications in different fields, from optoelectronics to sensing and actuators. Metal nanoparticles (NPs) are appealing due to their unique size, optical and structural features. Moreover, hybrid metal-semiconductor systems are particularly attractive, especially at the nanoscale, for the possibility of obtaining multifunctional materials, allowing for range of novel applications.
In this work, we report on the formation of metal Zn nanoparticles on the semiconducting ZnO surface by using the focused ion beam (FIB), an emerging tool for top-down prototyping allowing for patterning resolution down to the nanoscale. We show that, under appropriate conditions, it is possible to use ion beam based machining of ZnO crystals to induce the clustering of Zn ions and the consequent formation of metallic Zn NPs. The NPs formation is studied as a function of FIB parameters by means of SEM, AFM, Raman spectroscopy and TEM. Morphological investigation showed the gradual formation of protruding features with size of the order of few tens of nanometers. Fig.1a shows the AFM topography collected on ZnO surface after ion exposure. Raman spectroscopy allowed to identify the presence of metallic Zn and to study the dependence of the NP size on the ion dose. Transmission electron microscopy investigation (Fig.1b) and diffraction measurement revealed the presence of a shallow amorphous ZnO layer in which 5÷30nm-wide Zn particles with the same crystalline orientation of ZnO substrate are embedded.

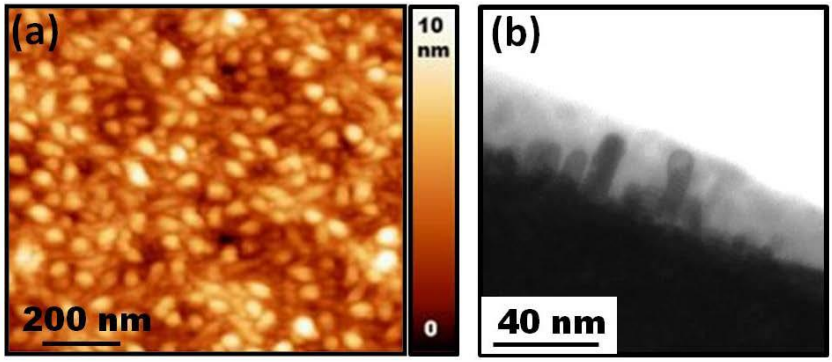

Fig.1: a) 2D AFM map and b) TEM micrograph of Zn NPs produced by FIB on single crystal ZnO.

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P22

Electrolyte gating of substrate-unbound nanowire-based devices

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Abstract:

Semiconductor nanostructures represent a promising platform for the exploitation of coupled electrical and thermal biases in thermoelectric devices [1]. However, the full benchmark of the thermoelectric figure of merit, *ZT*, in nanodevices, is not an easy task and typically resorts to challenging combination of optical and electrical techniques [2]. In particular, the need for *suspended* nanostructures to measure the thermal conductivity is detrimental to the field effect manipulation of the Seebeck coefficient. We fabricated semiconductor nanowire-based devices where the nanostructure is suspended approximately 200 nm over a SiO_2/Si++ substrate. The devices are equipped with a comb of electrodes allowing to measure the resistance of several sections of the nanowire. The latter is substrate-unbound, and this limits dramatically its capacitive coupling with the SiO_2/Si++ substrate, preventing to use it as a back-gate to modulate the electrical transport in the nanowire. This is particularly evident in the case of room temperature regime and degenerately doped semiconductor nanostructures. To overcome this limitation, we exploit ionic liquids as almost thermally insulating dielectric media for the conformal gating of suspended InAs nanowire-based devices, compatible with the nanowire thermal conductivity measurement via the 3ω-method [3,4]. The ionic liquid droplet surrounding the suspended nanowire-based device implements an electric double layer that efficiently gates the nanostructure in the temperature range from the liquid freezing temperature to room temperature. Noticeably, the selected ionic liquid is prepared free of contaminants and displays a wide electrochemical stability, thus we can operate the device within a gate voltage window exceeding 5 Volts at room temperature. Our results were reproduced for several thermal cycles from 300 K to 150 K, evidencing the mechanical stability of the hybrid ionic liquid-nanowire system and showing that the strain induced by the different thermal expansion coefficients does not represent a critical issue. Based on these preliminary results, we envision the realization of a universal device architecture for the all-electric measure of *ZT* in high aspect ratio nanoscale semiconductor devices.

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P23

Novel Pt/Ni/NiO based electrodes for electrocatalytic biodiesel production from palm oil

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Abstract
Over the last few decades, biodiesel has drawn increasing attention as a viable alternative to fossil fuel sources. The use of vegetal oils is of particular interest as a route to value potential waste-products for direct energy generation. In particular, palm oil is an edible oil, recently at the center of a lively debate about its usability for food purposes, leading to a substantial reduction in its market demand. Biodiesels are produced through transesterification of oils and fats glycerides with alcohol molecules. Transesterification is a typical two-phase reaction as a consequence of the poor solubility of the alcohol into the triglyceride phase. However, during the transesterification process water molecules are formed and undesirable saponification reactions may occur, reducing the yield and quality of the final product. Furthermore, the removal of unreacted catalysts requires extra purification steps. In order to overcome these problems, electro-assisted biodiesel production methods, in which catalyst is anchored on a support and water molecules are tolerated under certain limits, have been investigated. During the electrochemical route, the proton and hydroxide ions formed at the surface of the electrodes due to water splitting, enhance the reaction rate.
In this study, with the aim to exploit the high Pt catalytic activity, the facile preparation of Ni/NiO nanoparticles, as well as the combination of them, i.e., their intimate connection and synergism, a novel Pt/Ni/NiO-based nanocatalyst has been synthesized. Afterward, the as-synthesized nanocatalyst has been tested for the production of biodiesel from palm oil through a simple electrocatalytic process in an aqueous methanolic reaction mixture. The transesterification reaction occurred with a low amount of nanocatalyst in a two-phase reaction mixture where an emulsion of palm oil in the alcohol phase is formed under strong stirring. The effects of the applied voltage, reaction time and temperature on the methyl and ethyl esters yield were explored, and the reaction products were analyzed. High conversion rates, without saponification reactions for cell voltages below 25 V, and superior at ambient temperature, were found on the nanohybrid electrode.

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3D multifunctional carbon nanotube networks

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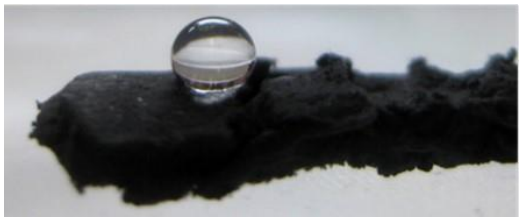
In the field of nanomaterials research, carbon nanotubes (CNTs), proved to possess unique physicochemical properties, owing to their nanoscale dimensions, that have been applied to improve the performance of existing processes or even design novel technologies.
Recently, there has been a growing interest in obtaining natural and synthetic three-dimensional (3D) architectures instead of two-dimensional ones to increase the active surface-to-volume ratio throughout the entire 3D structure, which proves to be advantageous in several applications. The 3D macroscopic structures can be obtained from the assembly of nanomaterials like graphene, carbon nanotubes, polymers and similar others, following chemical and physical routes and the resulting properties derive from the combination of those of the nano-constituents and those of the complex final architecture (like porosity, lightweight and others).



In this paper, we show that is possible to promote a direct self-assembly of CNTs to obtain 3D networks following a chemical vapor deposition route [1-3]. The self-supporting internal structure consist of interconnected CNTs and to lesser extent of carbon fibers that form a random skeleton with micrometer-size open pores. The porous nature of the network is directly responsible for its lightweight and the hydrophobic and lipophilic behavior, therefore the material is called CNT-sponge as shown in the figure. The macroscopic assembly shows high structural stability and good electrical conductivity, and mechanical response. The experimental results obtained in our laboratory, demonstrate that the 3D-sponge can be successfully applied as active material to address some environmental challenges involving water treatment [3], energy production [1], neural reconnection [4] and mechanical transducer.

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P25

UV-enhanced silicon detectors with zinc oxide nanoparticles acting as wavelength shifters

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Abstract:

Broad spectral response of photon detectors without cryogenic cooling is of great interest in many fields of application like spectroscopy and high-energy particle physics. In order to achieve it, different approaches can be found in literature. One approach is the multijunction detector incorporating different kind of absorbers. The drawback here is the fabrication cost as well as complicated fabrication technique [1]. Another approach is the application of wavelength shifters which absorb the UV light and re-emit it in the lower energy range which preferably matches the peak sensitivity of the detector. The application of chemical wavelength shifters like *e.g.* Tetraphenyl Butadiene (TPB) has been reported, but they posses some drawbacks like instability in contact with some substances and photo-degradation behavior [2]. There is also a concept of the application of luminescent nanoparticles on top of the detector, which act as wavelength shifters [3]. This approach has several advantages such as little interference in the detector structure (even the UV-blocking window of the detector does not pose a problem), straightforward deposition technique and large possibility of adjustment of the spectral regions depending on the kind of the nanoparticles. Thanks to the quantum confinement the absorption and emission properties of the material can be tuned. Other feature which has an impact on the emission and excitation properties are the defects, which can act as luminescent centers. The wavelength shifters considered for this application are two kinds of commercially available zinc oxide (ZnO) nanoparticles. The differences between them lay in the size and the structural quality, which influence their optical properties like emission and excitation spectra as well as photoluminescence quantum yield. For the application they are distributed in the poly (methyl methacrylate) – PMMA - matrix and spin-coated on the detector window. The work consists of the analysis of the parameters of the zinc oxide nanopowders as well as the nanopowders dispersed in the PMMA matrix. The problem has been investigated both theoretically and experimentally. The experimental part involved examination of the samples deposited on the laboratory glass and finally on the photodetector. Apart from the kind of zinc oxide nanoparticles, the technological parameters which were optimised was the concentration of ZnO in PMMA as well as thickness of the layer. Two types of photodetectors have been considered for modification: silicon photodiodes with broad spectral response from 190 nm to 1000 nm and Multi Pixel Photon Counters (MPPC) sensitive in the range 270 – 900 nm. These latter ones are used for sophisticated applications as well as single-photon detection. The comparison of parameters of the detectors before and after modification is shown.

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P26

From waste to biofuel: a new nano-carbo-catalyst

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Abstract:
Up to 80% of primary energy sources for transport, electricity generation and so on, come from fossil fuels. Their massive consumption is a well-recognized cause of major global pollution. Moreover, oil is a non-renewable and limited energy source, which is widespread used in a great variety of applications, from polymers to pharmaceutical products, too.
Hydrogen, natural gas, syngas and biofuel are regarded as new energy primary sources, among which biofuels have raised great attention due to the large availability of feedstock materials. Renewable feedstocks for bio-fuel production derives from plants residues, such as agro-forestry wastes, biomass and so on.
Valeric acid (VA) derivatives, in particular valeric acid esters, are considered a potential substitute to gasoline. VA can be regarded as an important intermediate in the industrialization of biofuels: it is typically obtained through catalytical hydrogenation of costless levulinic acid (LA), that, in turn, can be easily produced from hydrolysis of cellulosic biomass. Acid hydrolysis of cellulosic material is a widespread process in many industrial fields, from paper industry to nanocellulose (NC) production. However, strong acid environment could represent a major problem in LA post-treatment. Nevertheless, hydrogenation of LA to VA is, typically, carried out at high pressure, up to 30 bar, in presence of H_2.
Electrochemical catalytical hydrogenation (ECH) can represent a solid alternative to traditional heterogeneous catalysis, particularly, in combination to renewable energy power source (wind, solar…), e.g., because it does not require hydrogen and works at atmospheric pressure. Nanotechnology, over the years, allowed great improvements in the electrochemistry field, leading to more efficient and durable products. In particular, graphene and its derivatives are claimed to enhance electrochemical properties of nanoparticles, providing an optimal conductive support.
In this work, we report the synthesis of valeric acid from electro-reduction of levulinic acid, in presence of sulfuric acid, on a Sn/reduced graphene oxide (rGO) catalyst. The active materials for the electrodes was obtained by precipitation method and simultaneous reduction of GO. In particular, in this paper levulinic acid, present in wastewater derived from nanocellulose (NC) production, was used. Moreover, since VA is not soluble, after its production an easy separation and regeneration of the sulfuric acid solution can be obtained.

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Photoluminescence of Metal (II) Imidazolate complexes (ZIFs) for sensing alcohols

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Abstract:
Zeolitic Imidazolate Framework (ZIF), a sub class of Metal Organic Framework (MOFs), is a 3-dimensional nanoparticle consisting of metal ions and an organic linkers (imidazole). These cage like structure are porous and having topologies found in zeolites with high surface area. MOFs have shown to be a promising candidate in applications for nanosensors, gas storage and insulators. In this study, we report a rare example of cadmium-based metal-imidazolate framework nanoparticles which exhibits an intense blue luminescence. Different metal-imidazolate complexes (zinc (ZIF-8), cobalt (ZIF-67) and nickel) are also synthesised and these four complexes are characterised for their gas-absorption, photon-absorption and photoluminescent characteristics. Synthesis under identical conditions with different metals exhibits unique characteristics for each metal. The result is compared with commercially available Basolite Z1200® and it is shown that the Cd-based nanoparticles exhibit an intense luminescence, better than the commercial product. The Cd-based nanoparticles exhibit high luminescence response for ethanol and methanol compare to the Zn-based nanoparticles. These results reveal that these materials can be potential good luminescent sensor for detection of absorbed small molecules.

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A study of the external stimuli on hysteresis and electrical properties of TMDs-based field effect transistors

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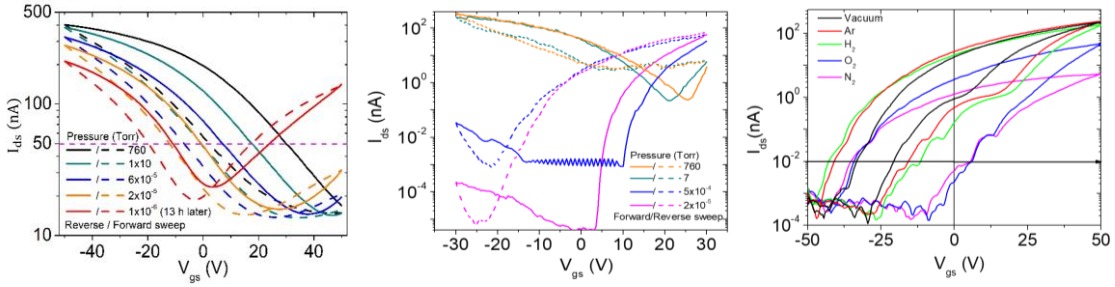
Abstract:

The control of n- or p-type behavior, as well as of the hysteresis, is an important prerequisite for the transistor exploitation in practical circuits. Indeed, even if hysteresis is in general an unwanted effect, a good control of pressure or gas on the hysteresis width can be exploited to create stable on/off states suitable for stable and no volatile memory elements.

In this general scheme mono and few-layer of CVD TMDs field effect transistors are studied under external stimuli (pressure, gas, electrical stimulations).

Exploiting the hysteretic behavior, we performed the characterization of MoS_2, WSe_2 and $PdSe_2$ under different environmental conditions varying the chamber pressure and gas atmosphere. We derive that for WSe_2 and $PdSe_2$ pressure enables both a modification of the hysteresis and a change of the type conduction, while for MoS_2 an ambipolar behavior cannot be achieved. Back-gated monolayer WSe_2 devices show a strongly dependence on the chamber pressure which tunes the conduction from p-type at ambient pressure to n-type in high vacuum [1].

Remarkably, we report a similar behavior for $PdSe_2$ devices increasing pressure by air in a time of a few minutes has a dramatic effect the transistor [2].



Graphs of the transfer characteristics as function on the pressure and gas (**left $PdSe_2$**, **center WSe_2**, **right MoS_2**).

On contrary, MoS_2 flakes measured in different pure gas environments do not show a modification of the type conduction either display an ambipolar behavior.

Different gas atmospheres define a change in hysteresis values, reasonably linked to the adsorption properties on MoS_2 surface and parametrized through the adsorption energy [3].

Comparison between different gases reveals that oxygen, nitrogen and hydrogen strongly act on MoS_2 electrical characteristic and in addition we proved that defective MoS_2 flakes are strongly influenced by non-polar gases like methane (CH_4).

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Investigation of Kinetic Functionals applied to metal nanoparticles

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Abstract:
In my work I develop advanced kinetic energy (KE) functionals for orbital-free density functional theory (DFT) applications. The KE functionals developed have tested on a newly developed benchmark which extend previous benchmark sets with bulk solids, kinetic potentials for OF-DFT, and absorption spectra of jellium sytems via the hydrodynamic approach. In the case I present a study of Laplacian-Level Kinetic Energy (KE) functionals [1] applied to metallic nanosystems [2]. The nanoparticles are modeled using jellium spheres of different sizes, background densities, and number of electrons. The ability of different functionals to reproduce the correct KE density and potential of various nanoparticles is investigated and analyzed in terms of semilocal descriptors. Most semilocal KE functionals are based on modifications of the second-order gradient expansion (GE2) or GE4 [3]. Gradient expansions are in fact powerful theoretical tools which describe with accuracy the KE slowly varying density regime of an electronic system, providing an ideal starting point for the development of approximate KE models. Semilocal KE functionals have the following form:

$$Ts[n]= \int dr\, \tau^{TF}(r)\, F_s(s,q,\ldots) \text{ where } \tau^{TF}=3/10\,(3\pi^2)^{2/3}\, n^{5/3}$$

is the Thomas-Fermi KE density and F_s is the KE enhancement factor.
The GE2 functional has the enhancement factor F_s GE2= 1 + 5/27 s^2 + 20/9 q where $s=|\nabla n|/(2*(3\pi^2)^{1/3}n^{4/3})$ is the reduced gradient with n being the electron density and $q=|\nabla^2 n|/(4(3\pi^2)^{2/3}n^{5/3}$ is the reduced Laplacian and the GE4 functional with its simplified enhancement factor has the form:

$$F_s \text{ GE4}= 1 + 5/27\, s_2 + 20/9\, q+\Delta \quad \text{with} \quad \Delta=8/81q^2-1/9s^2q+8/243s^4$$

I find that the Laplacian contribution is fundamental for the description of the energy (and potential) of nanoparticles.
Also I have tested a new formula (LAP1) with the following enhancement factor F_s^{LAP1}= 5/3 s^2 + $[1+(A-40/27)*s^2]/(1+A*\, s^2)*(1+3q+Cq^2)/(1+B*q^2)$ with A, B and C such that works better than the GE4.

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