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dear readers,

Dear Readers,

This E-nano Newsletter issue contains research highlights from the AtMol Integrated Project (EU/ICT/FET) and from top-level research institutions worldwide such as CIC nanoGUNE (Spain) or MANA/NIMS (Japan).
In addition, a detailed presentation of the one year EUPHONON coordination action started 2013 November 1st to establish a European community in Nanophononics is provided.
Detailed information about both projects, further reading documents and projects workshop series contributions could be found at www.atmol.eu & www.euphonon.eu
We would like to thank all the authors who contributed to this issue as well as the European Commission for the financial support (ICT/FET FP7 AtMol Integrated Project no. 270028 & ICT/FET FP7 EUPHONON Coordination Action no. 612086).

> Dr. Antonio Correia Editor - Phantoms Foundation

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editorial information

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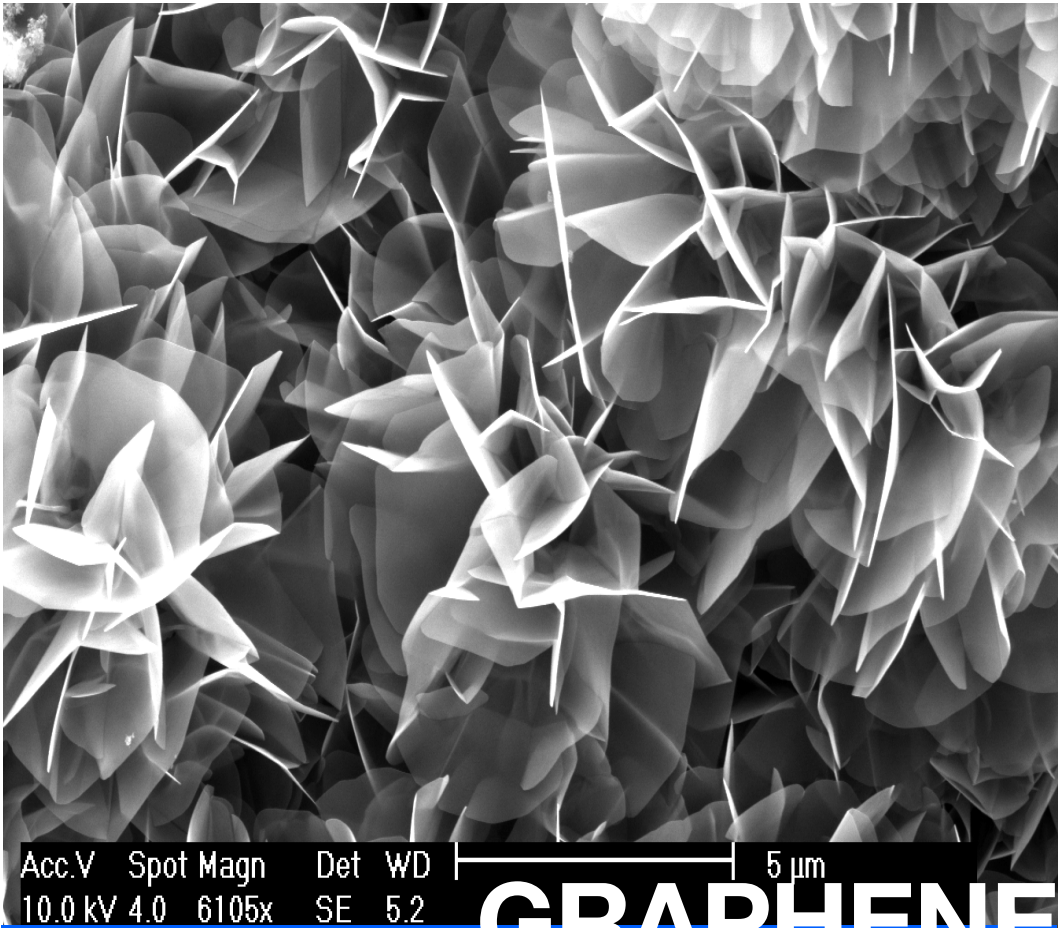

ON THE MOVE GRAPHENE

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EUPHONON-Building a European NanoPhononics Community: Presentation and goals

Sebastian Volz

Laboratoire d'Energétique Moléculaire et Macroscopique, Combustion, UPR CNRS 288, Ecole Centrale Paris, France

The one year EUPHONON coordination action started 2013 November 1st to establish a European community in Nanophononics with an emphasis on applications related to Information and Communication Technologies.

The two goals of the action are

(i) *to coordinate existing consortia in a wider community of scientists interested in ICT-Phononics* related initiatives by carrying-on at European level a well-structured activity composed by dissemination of scientific knowledge, networking of existing interest groups, production of position papers, tutoring and training future researchers and

(ii) *to propose to the European Community clear and supported evidences of the relevance of nanophononic fields for ICT* development in a common Manifest of communities that shares scientific and technological interests focused on NanoPhononics. The Manifest will have to establish the definition of the involved fields, then the list of available tools and foreseen applications. By answering to those questions, the Manifest will also provide a roadmap for coming ICT programs.

From the scientific and technological points of view, ICT devices must ensure basic functionalities like storage, retrieval, manipulation, transmission or receipt of information. In each of these functions, phonons have a key role:

Nanotransistors and hot spots. Incoherent phonons are the quantum quasi-particles of a solid that define their thermal properties when electrons are not involved. This is the case in a broad range of materials relevant to ICTs, such as semi-conductors. These phonons are of tremendous importance for thermal transport in nanodevices, where the temperature level is governing lifetime and reliability. For instance, nanotransistors involve electron currents crossing distances of about 20 nanometers and the efficiency with which electron energy relaxes onto optical thermal phonon defines the temperature of the generated hot spots [1-3].

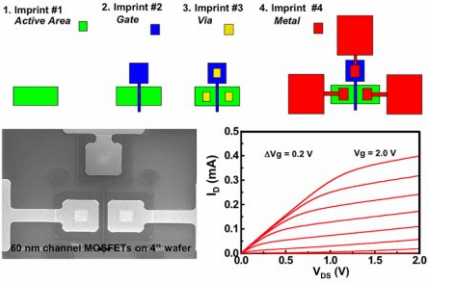

Fig. 1 > Schematic of the building blocks of a nanotransistor and its current vs voltage output (source: IBM)./

Phonons and Information Decoherence. Furthermore, the existence of a large population of phonons in a device is indeed a limiting parameter for information transport involving decoherence induced by phonons or electron-phonon interaction. The clear description of the

electron-phonon coupling mechanism is still an open question, whereas its impact is more than significant in today's 20-30 nm semi-conductor technologies [4-6].

Phonons and Electromagetic Field Noise. Thermal radiation has to be taken into account for the optimization of the ICT devices. Especially at frequencies in the Terahertz range, interactions between phonons and electromagnetic waves become important, e.g. plasmon-polaritons in ferroelectrics and multiferroics, phonon-magnon interactions in magnetic materials, and phonon-polaritons in polar media [7, 8].

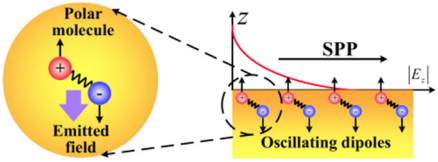

Fig. 2 > Generation surface phonon polaritons (SPP) by the fluctuation of electrical dipoles, which under a thermal excitation emit an electrical field that propagates along the material interface. These dipoles are spontaneously present in polar materials as SiO_2 and SiC./

Phonons as state variables? It is noteworthy that recent advances have been carried on the new concept of a "thermal diode" where thermal phonons are proposed to carry information like electrons in conventional electric circuits. More recently, concepts of thermal computation have been explored with a long-term perspective [9-11].

Acoustic Phonons and ICTs:
-*SAW devices* (Surface Acoustic Waves) are nowadays used in all mobile phones as SAW filters. For physical reasons intrinsic to SAW but also to technological electronic limitations, these SAW devices work in the GHz range. To go beyond the GHz limit, new devices manipulating and entangling electrons, coherent phonons, and photons must be planned [12-15].

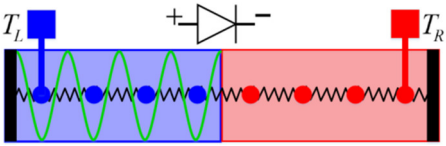

Fig. 3 > Schematics of a thermal diode to stop at or let thermal current through the interface depending on the temperatures T_L and T_R of the material segments. The right (red) segment is a chain of particles connected by elastic springs, while the left (blue) one is an identical chain but subject to a sinusoidal potential (green). If $T_L < T_R$, then the resonance frequencies of the red (blue) segment occur at low (high) frequencies (since the particles are confined in the potential valleys). Therefore, the vibration frequencies of each segment do not match and heat (which is the result of vibrations of the particles) cannot flow very efficiently. By contrast, when $T_L > T_R$, the particles can move freely between the barriers and thus their vibration frequencies partly extend to low frequencies, which matches those of the particles in the right segment. This match/mismatch mechanism makes directional thermal conduction, which is essential for building thermal switches and transistor./

-*Coherent control of phonons* allows the manipulation of the information (mediated either by photons or by electrons), which is an important function of ICT devices. The manipulation of electrons and/or photons in new devices requires a perfect control of the physical properties of coherent phonons inside the devices (frequency, polarization, focusing, phonon gain) [16, 17].

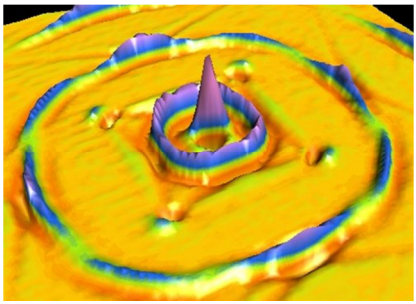

Fig. 4 > Experimental image of surface acoustic waves on a crystal of tellurium oxide./

-*Mega-to-GigaHertz*: Acoustics aspects have been addressed on one hand by the phononic crystal community relying on MEMS technology to actuate and detect Mega-to-GigaHertz waves. Localizing and clocking the acoustic waves in phononic materials opens indeed new perspectives for acoustic-based devices [15, 18].

-*Giga-to-TeraHertz*: a growing community is targeting GigaHertz-Therahertz acoustics, which corresponds to the generation, the control and the understanding of acoustics waves dynamics produced by ultrashort laser pulses (100 femtoseconds). Producing such high frequency coherent acoustic phonon opens the field of the nanoacoustics since the typical acoustic wavelength is included between tens and hundreds of nanometers [19, 20].

Opto-mechanics shows that it is possible to manipulate the vibrational state of micro- and nanostructures through the interaction with light (radiation pressure, photoelastic modulation, gradient forces in tailored geometries). Combining these interaction schemes with electrons and photons in photonic-phononic crystals and metamaterials at high frequency (>GHz) enables new functionalities and device concepts. Triggering light transmission (or reflection) with THz lattice vibration becomes now possible and is already addressed in the field of ultrafast optoacoustics. The opto-mechanics devices are also ultra-high sensitive force sensors based on the exchange of momentum and energy between phonon and photon at last. Therefore, opto-mechanics devices are even thought to play in the future an important role in quantum information processing technology [21, 22].

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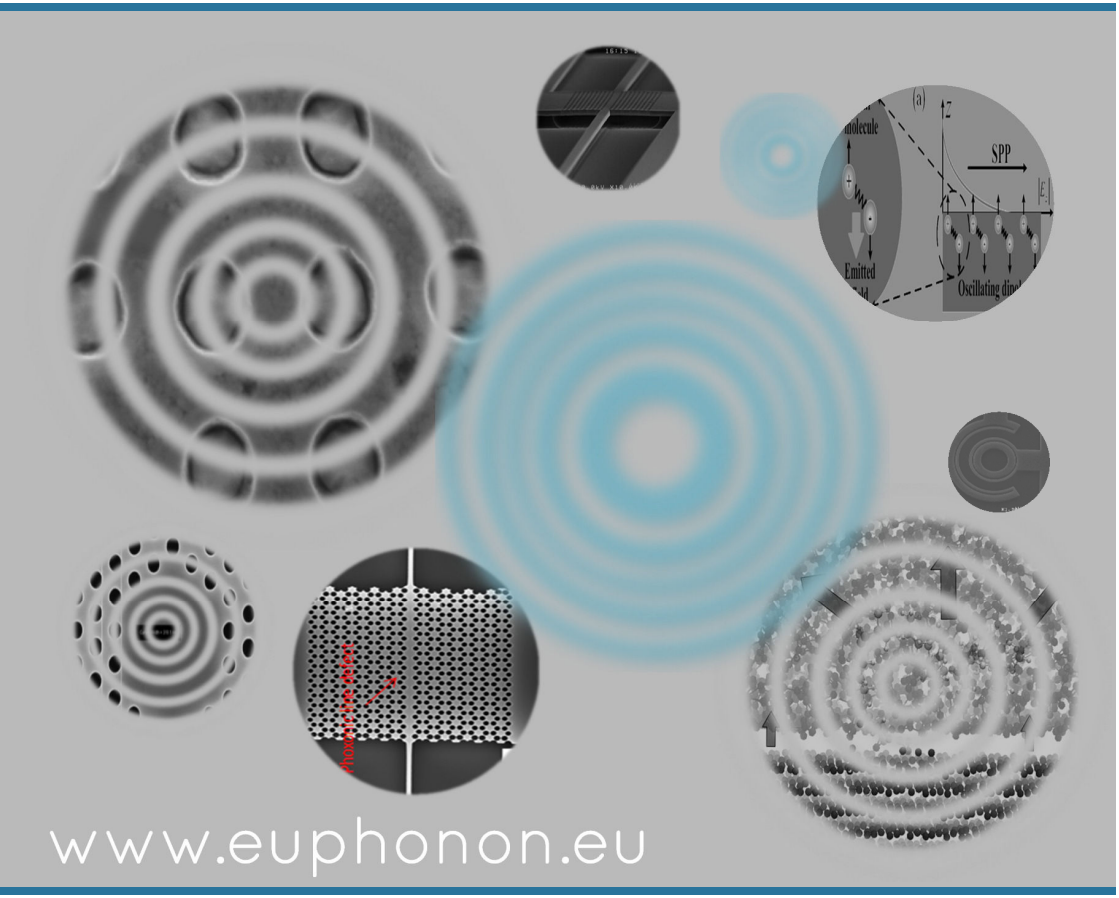
EUPHONON

Building a European NanoPhononics Community



consortium

Phantoms Foundation Spain

Teknologian Tutkimuskeskus Finland

Université du Maine France

CNRS France

Universität Konstanz Germany

Max-Planck Gesellschaft Germany

ICN Spain

EUPHONON project

The mission of EUPHONON, an EU-funded Coordination Action, is to gather communities working on (nano)phononics in Europe, identify the main research challenges impacting ICT and related sectors to advance our understanding and to explore the possible applications areas.

short facts

EUPHONON	Building a European NanoPhononics Community
EC contribution	400.000 euros
No. of partners	7
Coordinator	ECP-CNRS (France) / Prof. Sebastian Voltz
Running time	Nov. 01, 2013 - Oct. 31, 2014

EUPHONON events

Symposium "Phonons & Fluctuations in low dimensional structures" (Lille, France)

EUPHONON Workshop
(Le Mans, France)

further reading

nanoICT Position Paper on Nanophotonics and Nanophononics
www.phantomsnet.net/nanoICT/SRA

- N. Li et al. - Reviews of Modern Physics, 2012 – APS
- D. G. Cahill et al. - Applied Physics Reviews vol 1, 011305 (2014)
- E. Popo - Nano Research, Volume 3, Issue 3, pp 147-169 (2010)
- J. Cuffe et al. - Nano Letters 12 (7) 3569-3573 (2012)
- S. Volz (ed.) - vol. 107, Topics in Applied Physics, Springer 2010

nano phononics community

www.euphonon.eu/Reg

Project Summary

The aim of the EUPHONON project is to amalgamate the existing and future activities on phonon science and technology in Europe to establish a strong community in this emerging research field. The impact of EUPHONON will extend from academia to ICT-related industry by providing means for thermal management, optimisation of data handling and, in longer term, new methods for material characterisation and new paradigms for information processing. EUPHONON will set the definition for the phononics science and manifest the crucial goals in solid state physics, nanoelectronics and in bioscience in which the role of phonons has been overlooked. EUPHONON will create intimate collaboration between the various research fields, including theory, modelling, computation, information technologies and experimental science. A position paper on the importance and role of phonons will be one of the main outcomes of the project together with a research agenda, which could become the basis to guide, advance and prioritise the foci of the research resources in this field.

EUPHONON Objectives:

Nanophononics community building (mapping and benchmarking):

- To build and consolidate the emerging ICT-Nanophononics community
- To make the new European Nanophononics research community visible and prominent at both European and world scale
- To map research at European level and allow the identification of drivers/measures to assess research in ICT devices
- To network involving existing nanophononics national, regional or international activities/programs to exploit synergies, maximize impact and contribute to the definition of international cooperation strategies and/or the development of research collaborations

European Nanophononics Research Agenda:

- To define the scope of nanophononics, its tools, possible applications for ICT
- To document the findings and outcome of discussions in one position paper on definitions, tools, impact and applications
- To provide a Research Agenda to accelerate progress in identified R&D directions and priorities for ICT-Nanophononics-related FET program within Horizon 2020. This activity aims at guiding public research institutions and also at providing a valid source of guidance for Phononics and ICT industry (road mapping)

Dissemination of knowledge and outreach:

- To promote European research in ICT-Nanophononics related areas
- To disseminate knowledge and results

Project Main Goals

As a first step, a **Mapping of the Nanophononics community**, in this emerging area will be created. This database will allow a comparison of the scope and strength of the European community vis-à-vis those in other continents. The research coverage will be an element of the Research Agenda.

The consortium will organise a **Nanophononics Workshop** to present

the draft Research Agenda and obtain the feedback from the active researchers in nanophononics. It will allow extended discussions among researchers from the gathered communities to foster cooperation between them. The special emphasis of this workshop will be to refine Definition and Tools, following the release of the corresponding position paper and working documents on Applications and potential Roadmap.

A **Nanophononics Day** will be organised to spread the content of the initiative through Europe as an opportunity to increase awareness among the specialist communities in ICT as a whole.

In order to promote close collaborations with other international communities involved in activities related to phononics and to enhance the profile of FET at international level, a list of internationally renowned scientists in the field, including non-EU experts will be invited to join in the Research Agenda discussion. Scientists from academic research and industry will be invited to identify a selection of topics of interest and elaborate position papers.

EUPHONON position paper on Nanophononics to be released:

The Definition of Nanophononics in the context of ICT and specially future ICT will be refined by: surveying existing European related research communities, nanophononics related fields and key people, finding out the public and private R&D investments in Europe in nanophononics, refining considerations on ethical and societal impact, with possible public awareness and in consultation with learned societies, professional organisations.

The section on Nanophononic Tools will be prepared by: assessing progress so far in physical concepts, modelling and experimental methods, identifying the needs in tools, surveying publicly available computer codes to compute phonon properties of materials and phonon transport at an atomistic level (a key task will be to identify gaps in the landscape of software for nanophononics), monitoring novel conceptual approaches representing radical departures from the mainstream.

The section on Applications and Impact of Nanophononics will be prepared by: establishing the state of the art in technological achievements and scientific concepts with current hidden impact and prospective impact in ICT, carrying out a comparative analysis with the state of the art in the USA and Far East (strengths, weaknesses, opportunities, funding, etc.) with respect to applications.

Nanophononics Research Agenda:

Based on the findings of the Nanophononics Day and the Nanophononics Workshop, a Research Agenda will be prepared. It will contain statements emphasizing key scientific concepts and technological challenges to be developed under Horizon 2020 to keep Europe at the forefront in this emerging field of research and anticipate next ICT paradigms.

Draft Nanophononics Roadmap:

A Draft Nanophononics Roadmap will be prepared with a timeline and connections among topics. Considerations will be taken from the project findings and other major roadmaps.

Dissemination of knowledge and outreach:

A crucial activity of the project will consist of developing and maintaining a website aimed at widely disseminating results,

thus spreading excellence in order to promote European research in ICT-Nanophononics related areas and enhance collaboration among partners.

Euphonon Partners

CNRS: The Laboratoire d'Energétique Moléculaire et Macroscopique, Combustion, (UPR CNRS 288) involves world leading teams in the fields of Combustion and Transport Physics. Among those latter teams, the Thermal NanoSciences group headed by Sebastian Volz has developed a long-term expertise in the field of Nanoscale Heat Transfer in terms of physical computational modelling at macro-to-nanoscales. This covers phonon heat conduction in nanostructures and nanomaterials as well as near field radiation. In parallel, this group also proposed new nanoscale thermal metrologies based on Scanning Thermal Microscopy. More recently, thermoelectric and thermal interface materials are under focus.

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ICN2: The Catalan Institute of Nanotechnology (ICN2) is a research centre of the Generalitat de Catalunya. ICN2 has about 90 researchers. The 15- strong Photonic and Phononic Nanostructures (P2N) group is led by Prof. Clivia M.Sotomayor Torres and works on nanophononics (phonon confinement, nanoscale heat transport and phononic crystals in semiconductor, organic and oxide nanostructures). The group is constantly developing novel approaches and methods for nano-scale device-relevant research. It has pioneered research in nanofabrication (nanoimprint lithography, self-assembly and others) to realise 3D nanostructures.

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VTT: VTT Microsystems and Nanoelectronics is part of the VTT Technical Research Centre of Finland (Teknologian tutkimuskeskus VTT). The group is active in IC fabrication, MEMS, radiation detectors, thin films, RF-technologies, superconductors, nanoelectronics, nanophotonics, nanophononics and nanobioelectronics. The facilities include a 1900 square meter clean room of which 550 square meters is of class 10, equipped with 150 mm wafer processing line for BiCMOS and MEMS devices, thin film devices, nanoelectronics and micro and nanophotonics, wafer bonding, thinning and polishing processes, flipchip bonding and packaging. e-beam lithography up to 200 mm wafers, ALD, graphene CVD and nanoimprinting lithography.

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LEMANS: The Photoinduced-Dynamicsin-Condensed-Matter Group (DPMC) of the Institute of Molecules and Materials has a long-standing experience in ultrafast acoustics and optoacoustics. The scientific interests include fundamentals of laser-matter interaction and applied ultrafast acoustics aiming at controlling the photogeneration of coherent acoustic phonons by ultrafast light (photonphonon and electron-phonon coupling physics).

Acoustic nanowaves are used for directly probing the elasticity of nanostructures (studying acoustic eigenmodes of nanostructures, nanorheology, etc.). Colloids, semiconductors, nanoporous, confined liquids and correlated oxides are the systems currently under investigation.

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MPGP: The Max Planck Institute for Polymer Research (MPGP) of the Max Planck Society (MPG) is one of the world leading research centres in the field of soft matter, polymer and materials science. The Research Group for Nanostructures and Transport performs theoretical and computational research on the growth and aggregation mechanisms of nanostructures and nano-structured materials, and on their electronic and thermal transport properties. The group current focus is on assembly and thermal transport in carbon- and silicon-based nanostructures for electronic and thermoelectric applications. To this aim atomistic simulations, mostly based on molecular dynamics are performed and problem-inspired methodological development is undertaken.

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Uni-Konstanz: The Department of Physics os the Konstanz University is focussed on the physics of nanostructures, mesoscopic systems and nanotransport both in theory and experiment. The Modern Optics and Photonics Group (Prof. Thomas Dekorsy) is specialized in time-resolved femtosecond spectroscopy of coherent phonon excitation processes in different material systems and their nanostructures. The Nanomechanics group (Prof. Eva Weig) focusses on cavity nano-opto- and electromechanics, the origins of dissipation in nanomechanical systems, and integrated transduction schemes.

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PH: The Phantoms Foundation was established in 2002 (Madrid, Spain) in order to provide high level Management profile to scientific projects. The Phantoms Foundation focuses its activities on Nanoscience & Nanotechnology (N&N) and is a key actor in structuring and fostering European Excellence and enhancing collaborations in this field. The Phantoms Foundation plays an important role as a dissemination platform to spread excellence and increase the impact of Nanotechnology worldwide.

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www.phantomsnet.net

• PhD Position

Contribution to thermal microscopy by means of thermoelectric probe for nanostructures thermophysical characteristics quantification

Contact person: Laurent Thiery

laurent.thiery@univ-fcomte.fr

(FEMTO-ST Institute, France)

Deadline: September 13, 2014

Near-field thermal measurement tools represent a highly strategic field which exceeds by far the only problem of the imaging techniques. The measurement techniques of the temperatures and the thermal flows at short scales of space and of time are closely related to expected improvements in the field of the nanotechnologies.

• Job Position

Group Leader in nanotechnologies applied to food areas

Contact person: RRHH

reo@inl.int

(INL, Portugal)

Deadline: September 15, 2014

Applicants are expected to have an outstanding international research track record in one or several fields that are relevant in the current fields of research in nanotechnologies applied to food.

• PhD Position

Optical force & manipulation

Contact person: Manuel Nieto Vesperinas

mnieto@icmm.csic.es

(National University of Singapore, Singapore)

Deadline: September 17, 2014

• Job Opportunities (3)

Sales manager, marketing assistant, director of operations (PhD)

Contact person: Edurne de Pedro

d.marketing@nanoimmunotech.es

(nanoimmunotech, Spain)

Deadline: October 03, 2014

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• Job Position

Research Engineer position: Development of hybrid graphene/quantum dot photodetectors for image sensing applications

Contact Person: Frank Koppens

frank.koppens@icfo.es

(ICFO, Spain)

Deadline: December 15, 2014

ICFO – The Institute of Photonic Sciences, a centre based in Castelldefels (Barcelona, Spain), devoted to research and education of the optical and photonic sciences at the highest international level, is offering a research engineer position to a well-qualified, highly motivated and dynamic young scientist who wishes to enhance his/her scientific career in a friendly and stimulating environment.

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nanoresearch

Beyond CMOS: NANO-TEC project recommendations for research in nanoelectronics

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The NANO-TEC project held a series of consultative workshops on Beyond CMOS nanoelectronics to identify emerging nanoelectronic technologies, benchmark and analyze them in the frame of a SWOT analysis. Of paramount importance was the interaction with the design community towards the identification of ways in which a better interaction at the level of Beyond CMOS could help European research to make strides. A new methodology was developed for the benchmarking study. The consultation was extended to experts from the Americas and Asia. A summary of the recommendations is presented here.

Introduction

With scaling in CMOS technologies facing roadblocks in the next decades, research in the next technologies becomes a legitimate and urgent issue: Which are the most promising technologies? What do we need to know and understand in order to make informed choices? How to bring communities working on future technologies and in systems and integration together to enable Europe to convert this huge research potential in high-tech jobs and economic growth? In a nutshell, how do we strengthen the ecosystem technology-design in nanoelectronics in Europe?

Under the ICT theme of FP7, a Coordination Action, "Ecosystems Technology and Design for Nanoelectronics" (NANO-TEC, project number 257964, www.fp7-nanotec.eu), was funded by the European Commission with two main objectives:

- Identify the next generation of (emerging) device concepts and technologies for ICT.
- Build a joint technology-design community to coordinate research efforts in nanoelectronics in Europe.

I. Activities and Methodology

The main activity was based on interactive discussions during a workshop series. The four NANO-TEC workshops were: (1) *Identification of the main requirements for future ICT Devices*, Granada, Spain January 20–21, 2011, (2) *Benchmarking of Beyond CMOS device/design concepts*, Athens, Greece,13-14 October 2011, for which a special methodology was prepared, (3) *SWOT Analysis of the Technology-Design Ecosystem*, Lausanne, Switzerland, May 30-31, 2012, in which all the discussed technologies were analysed and (4) *Discussion of draft recommendations*, Barcelona, Spain, November 6-7, 2012, where the draft recommendations were discussed.

Overall 132 people participated in the NANO-TEC workshops, most of them more than once and several joining the

four workshops. The regional distribution was as follows: 92% Europe, 7% USA and 1% Asia. The corresponding affiliation types were: 45% academic, 40% research organisations, 11% industry and 4% policy makers and other stake-holders.

The discussions considered CMOS compatible technologies involving charge-based devices and their potential interface with this prevailing technology, other existing technologies and humans. Non-charge-based devices and emerging technologies were discussed in the general context of RTD. In general, the questions from the discussants attempted to ask the about the relevant parameter, for example, power and not speed, not necessarily a new switch but smarter switch, limits of binary computing, etc.

The **methodology** of the workshop was based on talks delivered by invited speakers on selected subjects and on the ensuing discussions. The strategy followed was first to consider a global nanoelectronics perspective, based on a thorough exercise carried out by the National Science Foundation and the Semiconductor Research Council in 2010 in which senior researchers from the USA, EU and Asia were involved. The topics included charge-based state variables, non-charge based state variables, new computing paradigms, ecosystem technology in Europe and progress in bridging the gap between technology and design.

Since one of the objectives of NANO-TEC is to strengthen the fragmented nanoelectronics community it was important that the workshop format would reflected objective. Hence, discussion time and effort were prioritised over extended presentations. As a result, it was decided that the workshops should consist of a mix of short presentations and goal oriented discussions.

A *discussant* was assigned to each speaker with the task of highlighting the key points of the talk and of raising challenging questions. This set the stage for group discussions in which all workshop participants were encouraged to take part. In addition, a *Rapporteur* was assigned to each topic with the task of documenting the presentation and discussion. During the second workshop, discussions were further enriched in parallel working groups focusing on the topics presented.

For the *benchmarking* exercise, a new methodology was developed in order not to exclude potential future functions while tracking common aspects, such as power consumption. During the *SWOT analysis* business niches and opportunities were identified.

Panels were organised to advance the discussions on building bridges between technology and design, in addition to specific presentations on design by invited speakers. Panel members presented their views in answer to specific questions, some prepared in advanced and others coming from the audience. The discussions were also documented in the records kept by the rapporteurs.

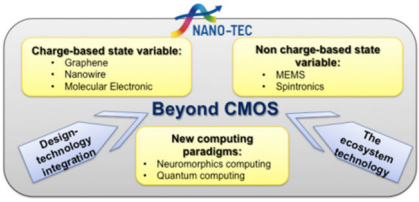

Fig. 1 > Schematic representation of the frame of reference for the 4th and final NANO-TEC workshop./

The second aim, i.e., bridging the gap in research between the communities of design and technology in Beyond CMOS was addressed in panel discussions and working groups as well as in specialist talks. In evolutionary RTD, a systematic approach to concurrent design and technology as a joint effort is not

uncommon. However, in the more disruptive RTD domain of Beyond CMOS, this joint design/technology learning curve has hardly started.

For the last workshop The interactions in the last workshop can be schematically represented as illustrated in figure 1.

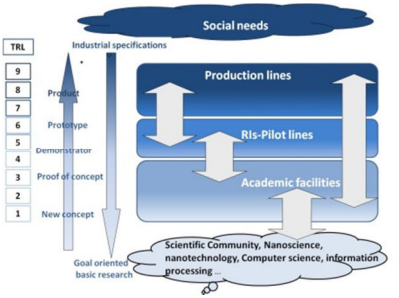

Fig. 2 > The ecosystem technology./

The presentations by speakers and discussants, rapporteur reports, working group material and workshop reports are all available to the public at: www.fp7-nanotec.eu.

Below, the recommendations of the project NANO-TEC consultation and associated activities are summarised. The full recommendations for each technology and the panel presentations, as well as the presentations by all speakers, discussant and rapporteur presentations, the working group conclusions, the benchmarking tables and the SWOT analysis are all available in the project web site public area. A report on each individual workshop may be also found there.

II. Summary of Recommendation

1. *Recommendations concerning R&D in state variables:*

- For *all state variables*, be these charge-based or not, it is recommended that research towards a better theoretical understanding of the underlying physics and material science of nano-scale devices is supported towards potential breakthroughs. In particular, the large variance in physical and electronic properties of the concepts and technologies discussed, requires that in addition to a higher level of knowledge, the design and emerging devices communities must work together to assess and exploit the full potential of this device- and system-relevant research area.
- Furthermore, *for most state variables*, the interconnect challenge at the nano scale, i.e., connecting to and from nano-devices, is a common one to be overcome theoretically, experimentally and technologically as it affects not only performance, interconnects and architectures, but also, and perhaps more importantly, reliability and temperature stability.
- Considering *charge-based state variables*, and in particular *nanowires*, it is recommended that a combination of nanowires technology with III-V compounds and or alternative architecture be explored with view to integrate III-V compound nanowire devices on a Si platform. In the area of *graphene*, emphasis should be placed on the suitability of fabrication and integration constraints in a combined Si-graphene new ICT technology, going beyond sensors and single components. Along the lines of two-dimensional systems, *layered materials* could be explored as alternatives as they exhibit an energy gap. In the light of recent progress, *topological insulators* should be considered earlier rather than later in a targeted research effort. The field of molecular electronics would benefit from strong collaborations between physicists and chemists on the one hand, with the technology and design communities on the other. Concerning *memristive devices*, local heating, which impacts

power consumption, needs to be addressed, as well as co-firing, fan-out and scalability bounds. Since highly non-linear processes are involved, work towards an adequate theoretical framework is mandatory.

- Concerning *non-charge-based state variables*, and starting with spin, it is recommended to support research in spin logic, as this constitutes a field, potentially able to deliver low power devices towards non-dissipative information processing. Any future program on *NEMS* should include a strong element on understanding contact physics, friction and wear at the nano-scale, all three factors being essential for the development of active power management and logic applications; further miniaturisation of NEMS through technology development, implementation of new materials and especially improved design and simulation tools to include several aspects of physics.

2. *Recommendations concerning R&D in new computation paradigms:*

- New computing paradigms are required for information processing including, for example, *neuromorphic computing, quantum computing*, chemical and molecular computing, quantum computing by molecular spin clusters and bio-inspired computing, among others. A practical recommendation in this field is to support research in a "super integrated project" or similar in which solid-state quantum computing and neuromorphic computing could become embedded in digital environments via digital-analogue hardware and software interfaces. The target would be to create useful hybrid systems to, e.g., interact with human users and be capable of adaptive learning. The research could be on fields in which unconventional computing could solve or give a more efficient answer in terms of energy consumption and computation time. Such a large collaborative and targeted project should pave the way for important commercial applications in five to ten years.
- It is recommended to continue the exploration of *novel computation approaches in general*. In particular, a *comparative and dynamic analysis of the interaction between design and the emerging computation technologies* as an integral part of the R&D efforts would provide Europe with a valuable and probably decisive advantage.

3. *Recommendations on the Design-Technology interaction:*

- This interaction is a challenging one. The consortium finds that strong motivation and support are needed in order to facilitate *communication and cooperation between design and technology actors* from academia and industry. These communities have very different cultures. In the course of this project, and during the project, progress has been made to establish communication and find some common terminology. Bearing this in mind, the consortium recommends that a couple of pilot projects are launched addressing explicitly not only the technical aspects but, above all, methodological aspects of this interactions with one or two well defined examples of novel state variables and a specific application each. The methodology lessons of such projects would be a starting point on the practicalities of meeting the technology-design challenge in Beyond CMOS research.
- A second recommendation is the setting up of a *simple and open infrastructure* for design connecting people and things. Such infrastructure

could have an international character beyond EU borders to allow free exchange of knowledge, where the "systemability" of 'Beyond CMOS' devices, which is a formidable challenge can be imaginatively addressed. Furthermore, modelling and simulation of 'Beyond CMOS' devices and circuits have to be developed to gain sustainable knowledge to feed in the design processes.

4. *Recommendation concerning the involvement of industry:*

- At present, the willingness of non-European industrial partners to enter in discussions on Beyond CMOS research has a higher profile than that of European ones. It is recommended that industry and researchers in Beyond CMOS intensify their interactions to define more clearly the expectations for future Beyond CMOS technologies, future needs and roadmaps of long-term research. An example of this would be to include technology readiness levels closer to the proof of concept one.

5. *Recommendations concerning research infrastructures and education:*

- The consortium recommends that measures are implemented to foster *the coordination of all technological facilities* having a significant activity in beyond CMOS research, in a European network preferably with a single entry point in each country. Crucial to the proposed modus operandi is common access rules and harmonisation of the organisational procedure, together with flexible financing support schemes facilitating smooth collaboration within Europe. The rationale is to take advantage of the complementarity of the Beyond CMOS research infrastructures and to capitalize on the fields of highest expertise in each country or region.
- The trend of the decreasing number of students in the physical and engineering disciplines did not go unnoticed. The consortium recommends that a multidisciplinary *Beyond CMOS* postgraduate training initiative be set up to educate a new generation of student in future information processing concepts, including theory of information, binary and non-binary information processing, as well as training the young scientists and engineers in Beyond CMOS technologies and design.

In summary, the NANO-TEC project has completed its cycle but much remains to be done specially in the area of enhancing and ensuring that a sound and timely interactions becomes a regular feature in European research in nanoelectronics, namely, a productive and stronger interaction between researchers in design and technology in Beyond CMOS nanoelectronics.

Acknowledgments

The authors are grateful to all members of the consortium, contributors, participants, speakers, panel members, discussants, working group conveners, rapporteurs and support staff for enabling the NANO-TEC project achieve its aims. The responsibility for the content of this paper rests with the authors. The support of the EU ICT project NANO-TEC (contract Nr. 257964) is gratefully acknowledged.

References

All the orignal reference material for all activities of the NANO-TEC project used to elaborate these recommendations can be found at: https://www.fp7-nanotec.eu/

The moment the individual pieces of the puzzle merge to provide the big picture.
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Flatland optics with graphene

* Researchers have developed an antenna-based platform technology for launching and controlling light propagating along graphene, opening new venues for extremely miniaturized photonic devices and circuits.

* They demonstrate focusing and bending of light trapped by the one-atom-thick material graphene.

* The work was published yesterday in the prestigious scientific journal Science.

Researchers from CIC nanoGUNE, in collaboration with ICFO and Graphenea, introduce a platform technology based on optical antennas for trapping and controlling light with the one-atom-thick material graphene. The experiments show that the dramatically squeezed graphene-guided light can be focused and bent, following the fundamental principles of conventional optics. The work, published yesterday in Science, opens new opportunities for smaller and faster photonic devices and circuits.

Optical circuits and devices could make signal processing and computing much faster. "However, although light is very fast it needs too much space", explains Rainer Hillenbrand, Ikerbasque Professor at nanoGUNE and the UPV/EHU. In fact, propagating light needs at least the space of half its wavelength, which is much larger than state-of-the-art electronic building blocks in our computers. For that reason, a quest for squeezing light to propagate it through nanoscale materials arises.

The wonder material graphene, a single layer of carbon atoms with extraordinary properties, has been proposed as one solution. The wavelength of light captured by a graphene layer can be strongly shortened by a factor of 10 to 100 compared to light propagating in free space. As a consequence, this light propagating along the graphene layer - called graphene plasmon - requires much less space.

However, transforming light efficiently into graphene plasmons and manipulating them with a compact device has been a major challenge. A team of researchers from nanoGUNE, ICFO and Graphenea – members of the EU Graphene Flagship - now demonstrates that the antenna concept of radio wave technology could be a promising solution. The team shows that a nanoscale metal rod on graphene (acting as an antenna for light) can capture infrared light and transform it into graphene plasmons, analogous to a radio antenna converting radio waves into electromagnetic waves in a metal cable.

“We introduce a versatile platform technology based on resonant optical antennas for launching and controlling of propagating graphene plasmons, which represents an essential step for the development of graphene plasmonic circuits”, says team leader Rainer Hillenbrand. Pablo Alonso-González, who performed the experiments at nanoGUNE, highlights some of the advantages offered by the antenna device: "the excitation of graphene plasmons is purely optical, the device is compact and the phase and wavefronts of the graphene plasmons can be directly controlled by geometrically tailoring the antennas. This is essential to develop applications based on focusing and guiding of light”.

The research team also performed theoretical studies. Alexey Nikitin, Ikerbasque Research Fellow at nanoGUNE, performed the calculations and explains that “according to theory, the operation of our device is very

efficient, and all the future technological applications will essentially depend upon fabrication limitations and quality of graphene".

Based on Nikitin´s calculations, nanoGUNE's Nanodevices group fabricated gold nanoantennas on graphene provided by Graphenea. The Nanooptics group then used the Neaspec near-field microscope to image how infrared graphene plasmons are launched and propagate along the graphene layer. In the images, the researchers saw that, indeed, waves on graphene propagate away from the antenna, like waves on a water surface when a stone is thrown in.

In order to test whether the two-dimensional propagation of light waves along a one-atom-thick carbon layer follow the laws of conventional optics, the researchers tried to focus and refract the waves. For the focusing experiment, they curved the antenna. The images then showed that the graphene plasmons focus away from the antenna, similar to the light beam that is concentrated with a lens or concave mirror.

The team also observed that graphene plasmons refract (bend) when they pass through a prism-shaped graphene bilayer, analogous to the bending of a light beam passing through a glass prism. "The big difference is that the graphene prism is only two atoms thick. It is the thinnest refracting optical prism ever", says Rainer Hillenbrand. Intriguingly, the graphene plasmons are bent because the conductivity in the two-atom-thick prism is larger than in the surrounding one-atom-thick layer. In the future, such conductivity changes in graphene could be also generated by simple electronic means, allowing for highly efficient electric control of refraction, among others for steering applications.

Altogether, the experiments show that the fundamental and most important principles of conventional optics also apply for graphene plasmons, in other words, squeezed light propagating along a one-atom-thick layer of carbon atoms. Future developments based on these results could lead to extremely miniaturized optical circuits and devices that could be useful for sensing and computing, among other applications.

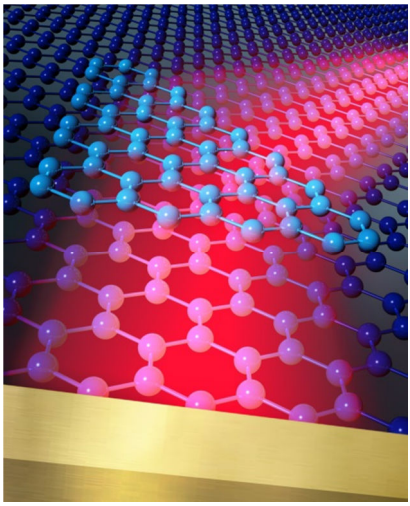

Fig. 1 > Graphic representation of the refraction of graphene plasmons - launched by a tiny gold antenna - when passing through a one-atom-thick prism (nanoGUNE)./

CIC nanoGUNE

The nanoGUNE Cooperative Research Center, located in Donostia-San Sebastian, Basque Country, is a research centre set up with the mission to conduct excellence research into nanoscience and nanotechnology with the aim of increasing the Basque Country's business competitiveness and economic and social development.

GRAPHENEA S.A.

Graphenea is a pioneer graphene production start-up company founded in 2010 by private investors and CIC nanoGUNE. The company produces and commercializes graphene films by Chemical Vapor Deposition technology and graphene powders by Chemical Exfoliation techniques.

ICFO

ICFO is a young research institution located in Barcelona that aims to advance the very limits of knowledge in Photonics, namely the science and technology of harnessing Light. Its research programs target the global forefront of photonics, and aim to tackle important challenges faced by society at large. ICFO is focused on current and future problems in Health, Energy, Information, Safety, Security and caring for the Environment.

Original publication

"Controlling graphene plasmons with resonant metal antennas and spatial conductivity patterns" Science (2014), DOI: 10.1126/science.1253202

P. Alonso-González[1], A.Y. Nikitin[1,5], F. Golmar[1,2], A. Centeno[3], A. Pesquera[3], S. Vélez[1], J. Chen[1], G. Navickaite[4], F. Koppens[4], A. Zurutuza[3], F. Casanova [1,5], L.E. Hueso [1,5] and R. Hillenbrand[1,5].

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Cover Image:
Graphic representation of the refraction of graphene plasmons - launched by a tiny gold antenna - when passing through a one-atom-thick prism.

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Nanomechanical sensors detect cancer from breath

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www.nims.go.jp/mana/research/highlights

An array of functionalised membrane-type surface stress sensors (MSS) distinguishes cancer patients from healthy people through a signature response to breath samples.

Cancer is the cause of 1 in 8 deaths worldwide, and early diagnosis can significantly improve survival rates. A collaboration of researchers in Switzerland and Japan has developed portable cancer detection units for non-invasive diagnosis. "We created an artificial nose that is sensitive enough to diagnose head and neck cancer through analysis of the breath," the researchers concluded in a recent report on their work.

The sensor design originates from conventional piezoresistive cantilever devices. Chemical layers coated on cantilevers absorb specific compounds and cause deflection of the cantilevers. These deflections can be measured through the change in electrical resistance at piezoresistors. However, these piezoresistive cantilever-type sensors have suffered from limited sensitivity. Recently, comprehensive structural optimization has led to a membrane-type surface stress sensor (MSS), achieving a significant improvement in sensitivity and stability. The MSS is composed of a thin silicon membrane (typically 2.5 µm thick and 500 µm in diameter) suspended by four piezoresistive beams attached to the circumference.

Frederic Loizeau at the Ecole Polytechnique Fédérale de Lausanne, Hans Peter Lang at the University of Basel in Switzerland, Genki Yoshikawa at the National Institute of Materials Science in Japan and their colleagues fabricated an array of MSS and coated them with different polymers to absorb various chemical compounds in breath samples. Reporting at the 26th IEEE International Conference on Micro Electro Mechanical Systems (IEEE MEMS 2013), the researchers presented that MSS could distinguish, in a double blind trial, the breath of four cancer patients from four healthy people.

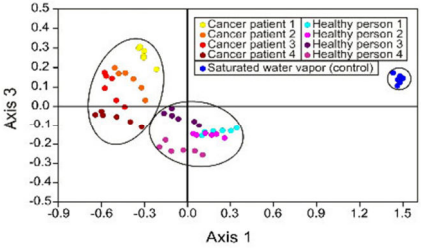

Fig. 1 > Principal Component Analysis case scores for breath samples of 4 healthy persons and 4 cancer patients. Each sample has been measured 6 times (colored dots). A breath sample bag containing saturated water vapor has been measured as a control (blue dots). Healthy persons can be clearly distinguished from cancer patients (the ellipses are a guide to the eye)./

Original publication

"Piezoresistive membrane-type surface stress sensor arranged in arrays for cancer diagnosis through breath analysis" 2013 MEMS 2013 621-624

Frédéric Loizeau[1], Hans Peter Lang[2], Terunobu Akiyama[1], Sebastian Gautsch[1], Peter Vettiger[1], Andreas Tonin[2], Genki Yoshikawa[3], Christoph Gerber[2] and Nico de Rooij[1]

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Revealing the "Scotch-tape" technique mechanism

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First In-Tandem Experimental and Theoretical Modeling of a Famous "Scotch-Tape" Technique for Making Two-Dimensional Graphene-like Nanosheets

The simplest mechanical cleavage technique using a primitive "Scotch" tape has resulted in the Nobel-awarded discovery of graphenes and is currently under worldwide use for assembling graphenes and other two-dimensional (2D) graphene-like structures toward their utilization in novel high-performance nanoelectronic devices.

The simplicity of this method has initiated a booming research on 2D materials. However, the atomistic processes behind the micromechanical cleavage have still been poorly understood.

A joined team of experimentalists and theorists from the International Center for Young Scientists, International Center for Materials Nanoarchitectonics and Surface Physics and Structure Unit of the National Institute for Materials Science, National University of Science and Technology "MISiS" (Moscow, Russia), Rice University (USA) and University of Jyväskylä (Finland) led by Daiming Tang and Dmitri Golberg for the first time succeeded in complete understanding of physics, kinetics and energetics behind the regarded "Scotch-tape" technique using molybdenum disulphide (MoS_2) atomic layers as a model material.

The researchers developed a direct *in situ* probing technique in a high-resolution transmission electron microscope (HRTEM) to investigate the mechanical cleavage processes and associated mechanical behaviors. By precisely manipulating an ultra-sharp metal probe to contact the pre-existing crystalline steps of the MoS_2 single crystals, atomically thin flakes were delicately peeled off, selectively ranging from a single, double to more than 20 atomic layers. The team found that the mechanical behaviors are strongly dependent on the number of layers. Combination of *in situ* HRTEM and molecular dynamics simulations reveal a transformation of bending behavior from spontaneous rippling (< 5 atomic layers) to homogeneous curving (~ 10 layers), and finally to kinking (20 or more layers).

By considering the force balance near the contact point, the specific surface energy of a MoS_2 monoatomic layer was calculated to be ~0.11 N/m. This is the first time that this fundamentally important property has *directly* been measured.

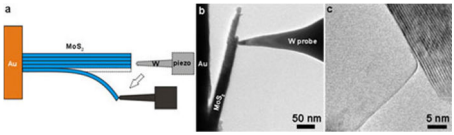

Fig. 1 > Nanomechanical cleavage of molybdenum disulphide atomic layers. (left) Schematics of the experimental setup inside HRTEM. (center) TEM image of a sharply etched tungsten nanoprobe in contact with the MoS_2 single crystal deliberately placed with (0002) basal atomic planes viewed edge-on. (right) HRTEM image of a cleaved MoS₂ atomic monolayer./

After initial isolation from the mother crystal, the MoS_2 monolayer could be readily restacked onto the surface of the crystal, demonstrating the possibility of van der Waals epitaxy. MoS_2 atomic layers could be bent to ultimate small radii (1.3 ~ 3.0 nm) reversibly without fracture. Such ultra-reversibility and extreme flexibility proves that they could be mechanically robust candidates for the advanced flexible electronic devices even under extreme folding conditions.

Original publication

"Nanomechanical cleavage of molybdenum disulphide atomic layers" Nature Communications, 5:3631 (2014) DOI: 10.1038/ncomms4631,

Dai-Ming Tang[1], Dmitry G. Kvashnin[2,3], Sina Najmaei[4], Yoshio Bando[5], Koji Kimoto[6], Pekka Koskinen[7], Pulickel M. Ajayan[4], Boris I. Yakobson[4], Pavel B. Sorokin[2,3,8], Jun Lou[4] and Dmitri Golberg[5]

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A cool approach to flexible electronics

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A nanoparticle ink that can be used for printing electronics without high-temperature annealing presents a possible profitable approach for manufacturing flexible electronics.

Printing semiconductor devices is considered to provide low-cost high performance flexible electronics that outperforms the amorphous silicon thin film transistors currently limiting developments in display technology. However the nanoparticle inks developed so far have required annealing, which limits them to substrates that can withstand high temperatures, ruling out a lot of the flexible plastics that could otherwise be used. Researchers at the National Institute for Materials Science and Okayama University in Japan have now developed a nanoparticle ink that can be used with room-temperature printing procedures.

Developments in thin film transistors made from amorphous silicon have provided wider, thinner displays with higher resolution and lower energy consumption. However further progress in this field is now limited by the low response to applied electric fields, that is, the low field-effect mobility. Oxide

semiconductors such as InGaZnO (IGZO) offer better performance characteristics but require complicated fabrication procedures.

Nanoparticle inks should allow simple low-cost manufacture but the nanoparticles usually used are surrounded in non-conductive ligands – molecules that are introduced during synthesis for stabilizing the particles. These ligands must be removed by annealing to make the ink conducting. Takeo Minari, Masayuki Kanehara and colleagues found a way around this difficulty by developing nanoparticles surrounded by planar aromatic molecules that allow charge transfer.

As the researchers conclude in their report of the work, “This room temperature printing process is a promising method as a core technology for future semiconductor devices.”

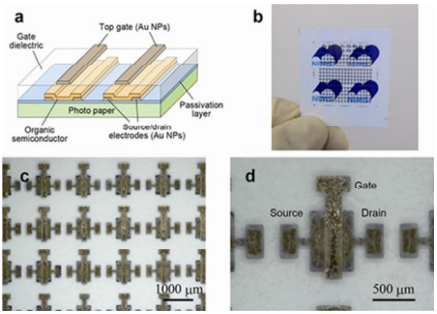

Fig. 1 > Fully printed organic thin film transistors (OTFTs) on a paper substrate. (a) Schematic of the device structure for a fully printed OTFT on paper. (b) Arrays of fully printed OTFTs fabricated on a paper substrate inkjet printed with the NIMS logo before adding the device. (c) An optical microscope image of fully-printed OTFT arrays. (d) A magnified optical microscope image of the individual device. Arrays of fully printed organic thin film transistors fabricated on paper substrates that had the the NIMS logo ink jet printed on before processing./

The gold nanoparticles had a resistivity of around 9 x 10^{-6} Ω cm – similar to pure gold. The researchers used the nanoparticle ink to print organic thin film transistors on a flexible polymer and a paper substrate at room temperature, producing devices with mobilities of 7.9 and 2.5 $cm^2 V^{-1} s^{-1}$ for polymer and paper respectively – figures comparable to IGZO devices.

Original publication

"Room-temperature printing of organic thin-film transistors with π-junction gold nanoparticles", Advanced Functional Materials, published online (2014).

Takeo Minari[1,2], Yuki Kanehara[3], Chuan Liu[1], Kenji Sakamoto[1], Takeshi Yasuda[1], Asuka Yaguchi[1], Shigemi Tsukada[4], Kei Kashizaki[3] and Masayuki Kanehara[3,4]

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We have now the technological knowhow to manipulate atoms and molecules one at a time on a passivated semi-conductor surface and to design elementary Boolean logic gates at the atomic scale using for example a few molecules adsorbed on this surface and interconnected by an atomic scale circuit, a single molecule embedding the complete gates or an atomic scale circuit alone (See Fig. 1). But how to determine which one of those directions will lead to a true revolution regarding the atomic-scale construction of the Arithmetic and Logic Units of our future processors?

First, there is a need to consolidate Atom Tech processes (Atomically precise Manufacturing) able to deliver from an initial native wafer up to the nano-packaging step what can be called a molecular chip that is chip whose active part is an atomic scale circuit embarking (or not) devices made of single molecule. AtMol partners have progressed a lot in this direction in the last few years introducing new UHV technology such as UHV transfer printing for fabricating nano-scale contacts free of resist [1] and nanoscale back interconnects for deporting the nano and micro scale wiring at the back of the wafer and for maintaining the atomic scale circuit and/or the molecule(s) at the top of the wafer [2]. More recently, the fusion between nanotechnology wafer fab processes and lab scale atom tech handicraft was established with the production of 200 mm Si(100)H wafers ready to be de-encapsulated in the UHV for STM atom by atom circuit construction or for interconnecting single molecules in a planar configuration and in the UHV [3]. Those processes are now completed by the fantastic progresses in atomic scale interconnection machines with the prospect to prepare multiple STM tip experimental interconnections at the top surface of an atomically prepared wafer [4, 5, 6].

Second, there is a need to determine the type of architectures adapted for the atomic scale and which of those architectures will be the most performant relative to power dissipation and to the calculation speed. Is it possible to construct a complex calculator based only on quantum mechanical behavior that is on exploiting the spontaneous time dependent answer of a quantum system prepared in a non-stationary quantum state? By increasing the circuit complexity, is it still necessary to have some gain here and there all along the circuit imposing many classical access to the quantum system because of the no cloning quantum theorem [7]? Quantum computer architecture (with or without qubits inside) are entering in the molecular electronic realm in a way to propose a miniaturized version of the actual mesocopic superconducting approach, of the statistical NMR solution approach, of the cold atom trap approach or of the embedded atomic scale impurities approach at the surface of a semiconductor [7].

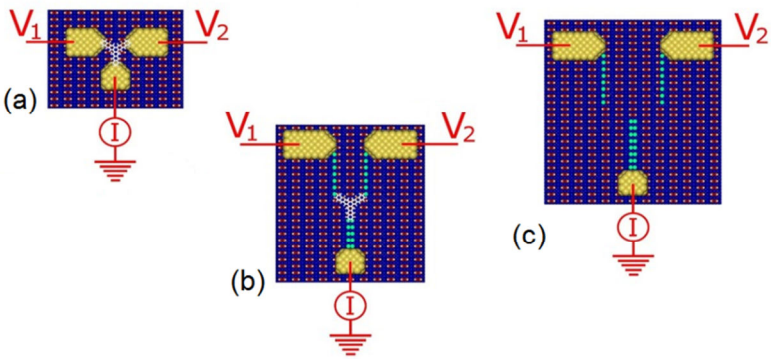

Fig. 1 > Schematically representation of the 3 possible terminals junction atomic scale OR gates constructed on a Si(100)H surface using metallic nano-pads interconnects (in yellow) as an intermediate between the central atomic scale structure of the gate and the interconnecting wires up to the macro-scale (represented by red wires for simplicity). The di-(9-amino,10-hydro-anthracene)[a, c]naphtacene molecule (in white) OR gate is adsorbed over 3 metallic nano-pads in (a) and over Si dangling bond atomic wires (lines of H vacancies, green atoms) in (b). The surface atomic OR gate circuit using only surface Si(100)H dangling bonds is represented in (c)./

Third, there is a need to determine what will be the best elementary unit embarking the functional elements for technology: molecule or atom circuits? Since the 1974 seminal paper by A. Aviram and M. Ratner [8], it was always taken for granted that a large molecule (or a well self-assembled set of molecules) will be able to do the job, that is to perform a complex logic function once properly interconnected or embedded in a single large macromolecule [9,10]. But in our days and after the fantastic progresses of single atom manipulation techniques, dangling bond circuits constructed atom by atom at the surface of a passivated semi-conductor surface may also be able to do the job instead of the molecular circuits at least in a semi-classical design [11].

Fourth, what about the performances (energy dissipation, computing speed) of an atomic scale calculator. The electronic resistance of a metal-molecule-metal junction is intrinsically large and may not be able to be lowered below a few 10 MΩ for a long molecule. Considering the stray capacitance of a molecular junction, the operational bandwidth of such device will not be larger than at best a few MHz. Surface dangling bond circuit may be a bit better with at best a few GHz if all goes well in the precision of the doping for the nanofabrication of the interconnection nanopads. Energy dissipation seems to be quite small for example adopting a simple architecting based on molecular scale switching elements, below 100 zJ per molecule switch [12].

Fifth, what is the best technology in term of sustainable development: Molecule(s) or atom circuits? In the 80's, a seminal paper by K. Ulmer put forward the question of the genome of a computer with the prospect to program genetically a bacteria for this bacteria to fabricate a nano-processor [13]. Is it still an actual paradigm or are we now so Cartesian that this paradigm disappears to the benefit of serious physics, chemistry and nanotechnology?

Following all those questions, the most actual one at work in the AtMol integrated project is the choice of matter: molecule(s) or atom circuits and a choice of material that is the best material for the wafer whose surface will be used to support and stabilize the atomic scale circuit? This debate is very active in AtMol and sometime the solution explored in AtMol are a mixt of the two [14]: the dangling bond atom wires to interconnect single molecule devices and even molecule latch to bring the logical input as close as possible to the atomic scale logic gates [15], the logic gate being constructed atom by atom on a passivated semi-conductor surface [11]. To present this AtMol internal debate to a large audience, we have selected 2 different points of views detailed here after: 1) the experimental exploration of the on-surface synthesis of elementary intramolecular circuits with the objective to establish and confirm quantum intramolecular electronic circuit laws and 2) the recent theoretical developments in the understanding of dangling bond wires constructed on a passivated surface with the objective to construct atom by atom the best conductive surface stabilized atomic wires. Theoretical understanding of intramolecular electronic circuit rules is also developed in AtMol together with the dangling bond atomic wires and logic gate construction. This was described in a recent AtMol workshop in Barcelona. The proceeding of this workshop had also been published [16].

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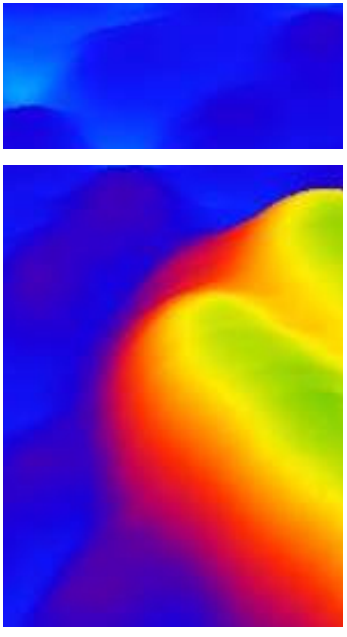
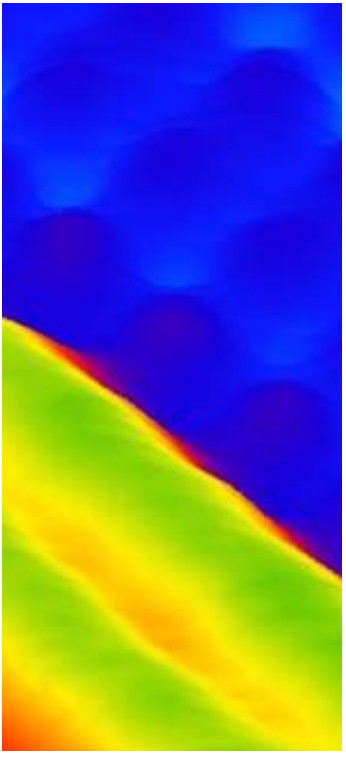
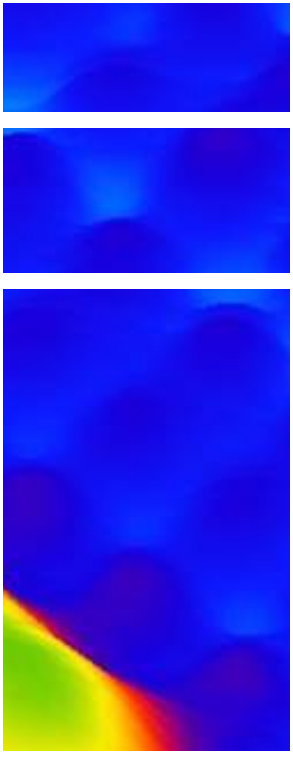

Atom by atom constructed dimer dangling bond wire on an Si(100)H surface

nanoresearch

Experimental approach towards molecular circuits

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An essential challenge in the field of molecular electronics is the construction of electronic devices based on the on-surface assembly of single functionalized building blocks. These functional units, supported by a surface, are connected to each other via molecular wires or atomic-scale wires. Such atomic scale circuitry should lead to better performances in terms of power dissipation and operation speed. In order to achieve this goal it is extremely important to gain fundamental understanding how to master the assembly of several atomic/molecular species into predefined architectures, possibly held together by covalently interactions in order to ensure high stability and enable efficient electron transfer between the molecular building blocks.

One strategy is the assembly of semi-classical intermolecular circuits on surfaces. The successful growth of such systems might allow to explore and verify the predicted circuitry laws that these nano-circuits obey. In the tunneling regime, semi-classical intramolecular circuits follow non-standard classical rules, due to the quantum character of electron tunneling [1]. This has been demonstrated theoretically (see Figure 1) [2] and was later used to design a semi-classical molecule OR gate with no molecular rectifier chemical groups [3]. In this regard, a first experimental verification of these laws has been reported recently [1]: Individual intermolecular circuits made of one and two identical paths in parallel have been synthesized *ex-situ* and their conductance was measured by a statistical break junction technique, confirming the role of interference in the conductance superposition law for an intramolecular circuit (Fig.1d). In AtMol and as a further progress in that direction, we are interested in probing the conductance through semi-classical logic gates circuits comprised of a central molecular node accessible via three branches (wires) as presented in Fig.1c.

Conventional sublimation methods are very limited in the deposition of complex molecular structures (as such a molecular circuitry) onto surfaces since these structures typically have a large molecular weight [4] that results in high sublimation temperatures, potentially above the decomposition temperature. Hence, it is very difficult – if not impossible – to deposit the molecular structures in an intact fashion under ultrahigh vacuum conditions. In this regard, we approached the surface assembly of molecular heterostructures by means of the on-surface polymerization technique [5].

The synthesis of covalently-linked molecular structures on a surface comprises the incorporation of specific, comparably weak intramolecular bonds in the monomer building blocks and the subsequent creation of reactive sites at these positions. This has been realized by the use of halogen–carbon bonds at specific sites of the molecules with lower

bond energies than the organic framework. The halogen atoms are dissociated by providing specific thermal energy, creating reactive sites at their positions in a controlled fashion without breaking other molecular bonds (the so-called activation step) [6]. The activated molecular building blocks subsequently diffuse on the surface and connect with one another by forming new covalent bonds [5]. The direct covalent-connection of aromatic moieties is advantageous to establish π-conjugation for efficient charge transfer [7] and in terms of robustness as well.

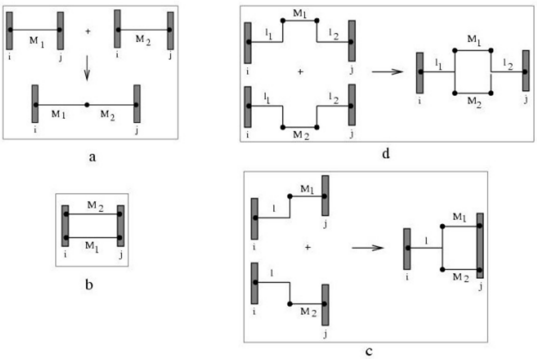

Fig. 1 > Simple single molecule circuit diagrams represented with their two contact nanopads metallic interconnects of the different series and parallel association of the molecular wires M_1 and M_2. The two molecular wires are: (a) bonded in series, (b) connected in parallel on the metallic pads, (c) forming a single molecule with one intramolecular node and (d) forming a single molecule with two intramolecular nodes./

The ability of molecules to selectively interact with each other plays a key role in nature and can be used for their bottom-up assembly on surfaces. It has been demonstrated that the topology of a molecular arrangement can be precisely engineered by properly designing and synthesizing the chemical structure of the elementary building blocks [8]. The number of active side groups per each building block, and the spatial arrangements of these interconnection points around the molecular framework are key points in determining the final molecular architecture. The position of the side groups has to be designed to maximize the interactions between the molecules and new covalent links, while steric hindrance must be suppressed. The subtle interplay between these features is essential for tuning the growth from one-dimensional structures, i.e. molecular wires for transporting information, or two-dimensional molecular networks (e.g. nanocircuits) [6].

In order that this procedure may efficiently work, it is important that the framework of each molecular constituent remains intact during the activation step as well. Furthermore, each individual molecule has to maintain sufficient mobility in order to diffuse sufficiently on the surface to hit other activated molecular species. At the same time chemical reactions between the activated molecular connection points and the surface itself must be avoided in order to preserve the availability of reactive molecular sites.

Incorporating different halogen substituents in the molecular building blocks as activating groups is a highly promising strategy in view of growing molecular architectures according to hierarchical covalent linking. The ability to activate dormant halogen bonds at different and well-defined activation temperatures opens up the possibility to better control the assembly process of molecules as well as the quality and the degree of complexity of multi-component molecular arrangements at surfaces [6]. Additionally, the surface structure

influences molecular diffusion and consequently the covalent linking of the building blocks. It has been shown that the use of stepped surfaces for the on-surface polymerization process does not only give insight into the catalytically active sites of the surface [9], but also can steer the linking reactions. In this way, aligned and parallel polymers as well as a higher polymer quality (in terms of size and defect number) are achieved [6,9].

The assembly of nanocircuits or hetero-nanostructures made of molecular wires and functional building blocks at surfaces is very challenging since the molecular recognition takes clearly place between different molecular species. A functional molecule (for instance a circuit node) must provide reactive side groups for the connection of a certain number of wires. The molecular species has to be designed in a way that the chemical recognition is maximized between the two species in order to efficiently prepare these nanocircuits (in contrast to a segregation process if mixed structures are unlikely formed [6]).

Finally, a way to probe the circuitry laws followed by these nanocircuits is by means of the scanning tunneling microscopy (STM) pulling technique [4]. The STM allows to identify and image specific nanocircuits with submolecular spatial resolution. The circuit conformation within the STM junction as well as the whole environment around the nanostructure can be fully characterized at the atomic scale, unlike typical break junction experiments where the transport information through the single molecule is extracted from a statistical analysis without detailed information about the surroundings [10].
Once an individual nanocircuit is identified, the STM tip will be placed on top of a wire´s end (at disables STM feedback loop) and approached until a robust contact is established. Then, the tip is retracted, the circuit is lifted up and the conductance measured as a function of the vertical tip displacement (I(z) pulling curve) [7]. This shall open the possibility to investigate and isolate the contribution of a single functional groups to the measured conductance by STM imaging of the molecular nanostructure before and after the process. At the same time electron transfer can be explored through simultaneous pathways in the case that a functional unit (e.g. a molecular node) is connected to more than two wires. This should open the possibility of probing expected interference effects when tunneling through a single molecule.

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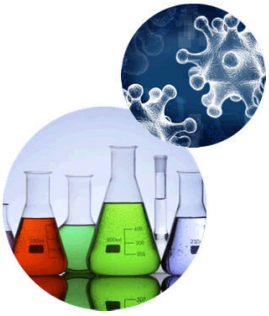

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Surface atomic wires for interconnects and logic gate design

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Introduction

The development of information technology has been pursued at a tremendous pace. Larger capacity memories and faster processors are obtained from the miniaturization of electronic devices. Nevertheless, this technological explosion that started in the second half of the 20th century will reach a limit when facing the atomic scale. Indeed, at this size, the bulk properties of semiconductors are modified. Thus, the operating principles will vanish along the shrinking process [1,2]. In the mid-1970s, an alternative was offered by proposing that a single molecule could perform the same basic functions of electronics than traditional silicon-based technologies [3,4]. In this purpose, organic molecules are candidates with great potential given the control on molecular design rending possible by chemical synthesis. In particular, one can conceive molecules that will switch from one state to another under the application of some external stimulus [5]. When this bistability is associated with a response function (e.g. optical), binary data can be encoded following the same rules that served in traditional devices. Then the logic operations, either basic (AND, NOT, OR) or more elaborated can be performed at the molecular level, giving rise to molecular logic gates [6,7,8,9].

Semiconducting surfaces are good candidates for supporting the running of molecular devices because they have an electronic gap that prevents current losses from the device plus their surfaces present localized chemical bonds that make them ideal to attach a molecular device. However, semiconductors are generally doped, and dopants can be a source of nuisance to the operational conditions of the device. On one hand, they are strong electron scatterers, perturbing transport properties in a very long-ranged manner, and, on the other-hand, they can close the semiconductor's gap. One remaining problem is to create a frame, at atomic scale, where a number of these 'molecular processors' could be (i) assessed, and (ii) associated together to obtain complete circuits.

Atomic Wires on Semiconducting Surfaces

It has been shown that atomic scale circuits can be obtained using the scanning tunneling microscope (STM), which can selectively remove atoms on the surface of semiconductors to construct lines [10,11,12,13,14,15,16]. The dangling-bonds (DBs) created by the removal of atoms introduce then states in the band gap of the semiconductor. An important example of such fabrication is the DB wire produced by the selective removal of hydrogen atoms from an H-passivated Si(001) surface along the Si dimer row (see Fig. 1).

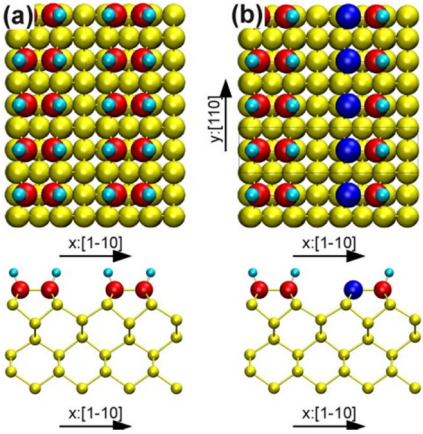

Fig. 1 > Atomic structure of (a) the Si(100)-(2x1)-H surface, (b) the infinite ideal wire drawn along the y direction. H atoms are depicted in cyan, while Si atoms are depicted in red (surface dimers), yellow (others) and blue when holding a dangling-bond./

This DB wire has a single dangling bond per Si atom, offering a 1D metallic band within the gap. The transport of such a wire has been previously inspected by Extended Hückel calculations and a tight-binding model [17,18]. Unfortunately, the later configuration is not stable and a Peierls distortion takes place, involving a metal-insulator transition. The unstable DB wire, referred to as the ideal wire in the following, can also relax in two magnetic forms resulting from the antiferromagnetic and ferromagnetic coupling of adjacent DBs, respectively. The description of these different states has been the subject of intense activity thanks to density functional theory (DFT) based calculations [19,20,21,22,23,24,25,26,27]. In particular the magnetic solutions appear to be more stable than the distorted structure, referred to as the non-magnetic (NM) wire, when dealing with finite-size wires [25,27]. Although these relaxed periodic structures break the metallicity of the DB wire by opening a gap, it does not dispose of the possibility to find transport through a finite wire of DB.

A. Dangling-bond wires

As we just saw, dangling-bond wires are ideal candidates to craft atomic-size circuitry on the surface of a semiconductor, for example Si (100). As shown in Fig. 3a, the completely hydrogenated Si(100) forms a (2×1) reconstruction by the creation of dimer rows along the y:[110] direction. A DB-wire can be constructed along two perpendicular directions, as we remove a line of hydrogens along the dimer rows direction (y), or perpendicular to it (x:[1-10]) (Figs. 3b and c, respectively). The band structure of the system is shown in Fig. 2a. With dots we show the bands with weight from the DB silicons. We can observe that two bands appear in the bulk energy gap, and they mainly come from the DB-silicons. The gap is reduced with respect to the completely passivated surface, but we still obtain 0.66 eV for the direct band gap, and 0.50 eV for the indirect one. Hence, despite of introducing many electronic states in the gap of Si, the relaxation of the atomic structure leads to opening of a gap and thus, to worsen the possible transport properties of the DB wire. Besides geometrical (Peierls distortions) relaxation

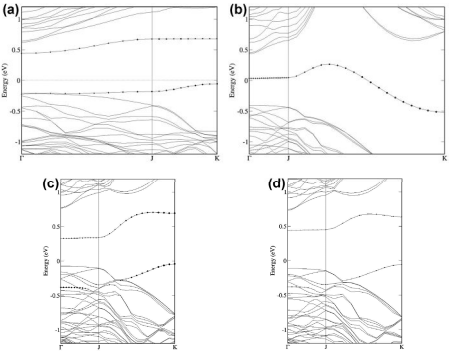

Fig. 2 > Electronic bandstructures of several DB-wires: (a) wire in the x-direction; (b) wire in the y-direction using the (4×1) unit cell (ideal case); wire in the y-direction using the (4×2) unit cell in the NM distorted (c) and AFM (d) situations./

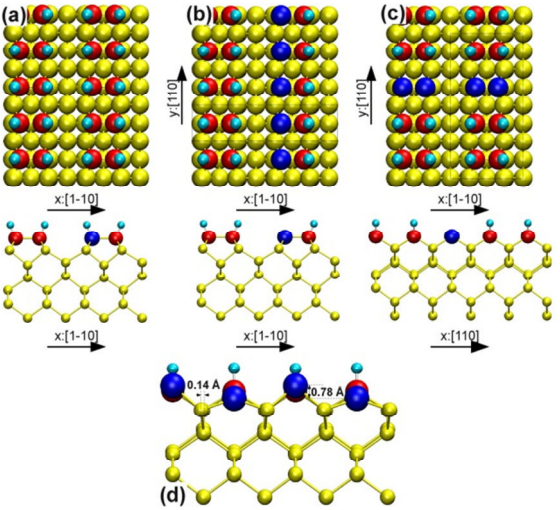

Fig. 3 > Cartoons of the completely hydrogenated Si(100)(2x1) surface (a), and DB-wires in y:[110] (b) and x:[1-10] (c) directions are shown. In (d) we show the Peierls-like distortion of the DB-wire in the y-direction when using a (4×2) unit cell. Cyan balls represent hydrogen atoms, while silicon atoms are represented by red (surface dimers), blue (Si with dangling-bonds), and yellow (all the rest) balls./

of the DB wires, there can be magnetic solutions that also lead to opening of electronic gaps. Ferromagnetic (FM) and antiferromagnetic (AFM) couplings between the atoms in the DB wire shows that indeed other solutions exist. The FM case is less stable than the ideal DB-wire by 27 meV/DB, and hence it will not be more stable than the Peierls distorted wires. However, the AFM one is more stable by 41 meV per DB. Each Si atom in the DB-wire has a magnetic moment of 0.50μ_B, and couples antiferromagneticaly to its neighbors in the wire. In Fig. 2d we show the band structure of the system. It is similar to the distorted case (Fig. 2c), with a direct (indirect) band gap of 0.55 eV (0.50 eV). In this case the occupied band has contributions from the majority spin of one silicon atom in the DB-wire, and the minority of the adjacent, while in the unoccupied band we find the minority spin of the first atom, and the majority of the second. Hence, DB-wires on passivated Si (100) may not be a good strategy for interconnect creation since the stabilization of the wired under electron-phonon and electron-electron interactions lead to gap openings and to either Peierls-distorted or antiferromagnetic solutions. The opening of a gap is clearly destructive for the low-bias transport operability of such an interconnect.

B. Surface-state engineering strategies for atomic-size interconnects

However, there are strategies that lead to an improvement of the transport properties of DB-based interconnects. These strategies are based on different arrangements of the nanowires are explored since the cause of the above large correlations can be traced back to the confinement of the electronic structure of dangling bonds. Hence, arrangements that allow for more extended electronic states, should in principle reduce electronic correlations and generally improve charge transport properties. Here, we study three arrangements and we compare them with the results of the strongly correlated case of a single-row dangling-bond wire, Fig. 4 (a). The first attempt is to increase the charge delocalization by increasing the inter dangling-bond distance. Here the hope is that hybridizations are still large enough while reducing the electronic Coulomb repulsion. The corresponding half-row wire is shown in Fig. 4 (b). Another arrangement is shown in Fig. 4 (c), the zig-zag wire that is a mid-case between the previous single-row and half-row wires. Finally, Fig. 4 (d)

considers the effect of increasing the density of dangling-bond states to reduce electron localization. As expected correlations efefcts are reduced due to the larger extension of the electronic structure and the charge transport properties of the zig-zag and double-row wires are very much improved. Our study concludes that, in particular, zig-zag nanowires can be an interesting alternative to surface interconnects.

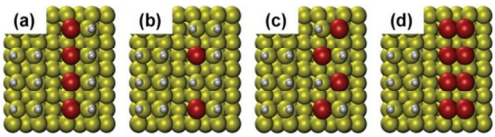

Fig. 4 > Atomic structures of (a) the single-row, (b) the half-row, (c) the zig-zag, and (d) the double-row dangling-bond (dangling-bond) wires. H atoms are depicted in white, Si atoms in yellow and red when holding a dangling-bond./

C. The role of dopants: current leakage

As we have seen, an interesting material to study the effect of dopants is silicon. Silicon-based atomic-size circuitry has been rapidly progressing from new proofs-of-concept of devices to single-atom quantum dots, based on surface silicon dangling bonds (DB) 28 and new structures formed by DB quantum dots with qubit capabilities. 29 Arrays of aligned DB have been shown to present specific electronic properties, 30, and we have explored above their properties as surface interconnects. In this context, dopants can severely impair the capacity of holding the electrical current to the interconnect: the current may leak from the wire. In traditional transistor-based circuitry, the leakage of current through the gate dielectric is actively studied. 31 However, the new interconnects lead to another type of current leakage due to the coupling of the DB wires to their environment: indeed the overlap of DB electronic states with bulk Si bands, allows the transfer of electrons initially confined to the wire, into the bulk material, hence losing them. Boron and phosphorous atoms replace a Si atom and create p-doped and n-dope regions, respectively, in Fig. 5. By placing the dopant at different distances from the wire, we can test the extension of the effect of the dopant in the current leakage. In order to avoid the reconstruction of the wire into a distorted one [12,21,25,32,33], we use the coordinates of the passivated surface. In Fig. 5, we see three different combinations: (a) only the contact region (*ii*) is doped, (b) there are dopants in the three regions, or (c) the dopants lie in two regions, one of them being the contact region (*ii*). These combinations allow us to calculate different currents. The system of Fig. 5 (c) contains an undoped electrode such that for low bias the only conduction channels belong to the nanowire. In this case, the current is entirely held by the DB wire since there is no other possible conduction path for the electrons entering the undoped electrode. This setup acts like a filter that selects the electrons that flow through the DB wire as the only ones forming the current. We call this contribution I_{filter}. In Fig. 5 (b) there is no restriction and holds a total current I_{total} that is composed of a dopant current contribution I_{dopant} and the DB wire contribution I'_{filter}. In Fig. 5 (a) the current is confined to the nanowire except where the transport channels are perturbed by the presence of dopants. This is the contact region where an extra contribution $I_{impurity}$ can be found. Setups (a) and (b) are the same setup in two different doping limits: the single impurity or dopant limit for case (a) and the massively doped case (b). In the absence of dopants, the current will just be the full nanowire's current that we take as the current reference, I_{ref}, since it is the maximum current the nanowire can convey. Then the leakage current will *be* $I_{leakage} = I_{ref} - I_{impurity}$ for (a) and $I_{leakage} = I_{ref} - I_{filter}$ for (b) and (c).

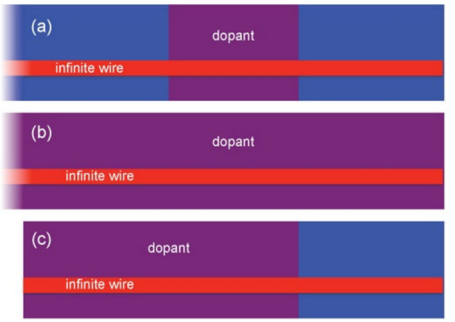

Fig. 5 > Scheme for the atomic structures that held a wire over three different Si surface region: two semi-infinite electrodes and a central connecting region between the electrodes. In (a) only the central region is doped, in (b) there are dopants in the three regions, and in (c), dopants are found in two regions, one being the contact region./

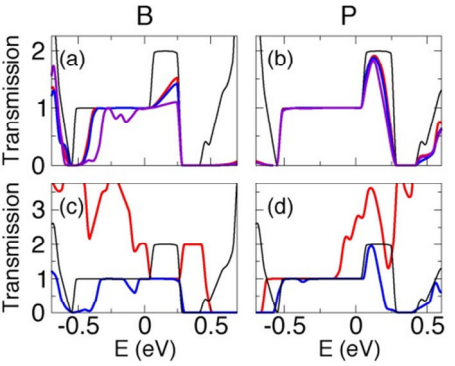

Fig. 6 > Electron transmissions as a function of electron energy. In the absence of dopants, the transmission is shown in black. (a) Single substitutional dopant, made by a B-atom located at 15 Å (red curve), 9.5 Å (blue curve), and 4 Å (mauve curve) underneath the nanowire. (b) Single substitutional P-atom for the same distances and color code as in (a). (c) Massively doped system with B-atoms in the left electrode plus contact region (blue line) and also in the right electrode (red line), the dopants are located at 4 Å underneath the nanowire. (d) Same as (c) but using P-atoms./

A key quantity in our calculations are the electron transmission, T(E,V), at a given energy, E and for a system bias, V . Figure 6 shows the transmissions at zero bias. Here, we assume that the interconnects are long enough to present a minimum electric-field effect, even if the biases get substantial. In the first panels of Fig. 6 (a) and (b) we find the results for B-doped substrates, and on (c) and (d) for P doping. As the impurities move away from the wires, the transmission changes,but within the used distances (15, 9.5 and 4 Å) the qualitative behavior is the same. Figure 6 (a) for a single impurity and (b) for a massively-doped substrate, shows that for B impurities the negative-energy transmission is very affected. This is due to the interaction of the DB wire's electronic structure with the energy levels of the B ion itself. At positive electron energies, there is also substantial damaging of the transmission and indeed a full transmission channel disappears as our transmission eigenchannel analysis 34 shows. For P impurities, (c)-single impurity and (d)-many impurities, the higher-energy levels of the impurities leads the main effect to positive energies. Indeed, P ions perturb the transmission less than B ions because the initial impurity levels lie further away from the Fermi energy. Hence, a lower leakage current for devices adsorbed on n-doped samples is expected. Blue curves correspond to setup (b) and red to (c), they are then the nanowire transmission and nanowire plus dopant transmission, respectively. A lot of information can be gleaned by studying the electronic levels of these systems. By computing the energy bands in a fully periodic system, we can obtain these energy levels. And indeed we obtain that the cause of the current leakage is the mixing of DB states with bulk states. In this way, DB states are not confined to the substrate anymore, and an electron transmitting through the surface DB's has a finite probability of ending up in the bulk material. We have computed the fraction of

the current that the wire holds that goes into bulk states. This is a measure of the leakage current or the current that is lost by the interconnect due to its coupling with the environment. The above two limits of dopant concentration yield qualitatively similar results, stressing the strong perturbation that a single dopant can exert on an atomic-size wire. Our calculations permit us to conclude that n-doped Si will be less leaky than p-doped Si. For the low bias at which these nanodevices will operate, leakage currents will be less than 10% for n-doped Si substrates, and 20% for p-doped ones.

Conclusions

In order to reach the atomic scale limit of nanodevice designs, different concepts and techniques must be mastered as listed in the AtMol Editorial of thie e-nano issue. In the present article, we have reviewed the on-going efforts trying to design optimal atomic scale interconnects for molecular devices and may be one day for dangling bond logics. We have analysed the awaited properties of DB wires. At the same time, the core of the molecular device will be represented by the functionalities that can be built in logic gates. It remains to confirm experimentally the electronic and ballistic, pseudo-ballistic or tunnel transport properties of those dangling bonds Surface atomic wires.

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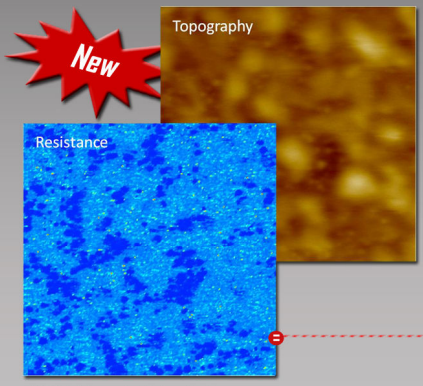

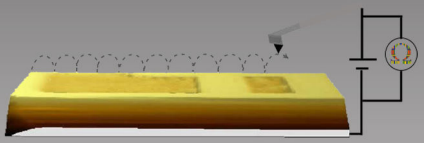

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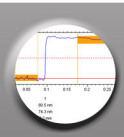

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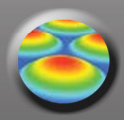

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