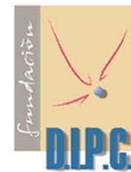


3rd Spanish - March 2006
Paperion Workshop



DONOSTIA INTERNATIONAL PHYSICS CENTER



On behalf of the Honorary, Advisory and Technical Committees, we take great pleasure in welcoming you to Pamplona for the third meeting of the Spanish Nanotechnology Network NanoSpain.

During the last two decades, a revolutionary scientific new age, based on the capacity to observe, characterise, manipulate and organise matter in the nanometric scale, is appearing. In this scale, physics, chemistry, materials science, computational theory, and engineering converge towards the same theoretical principles and experimental findings that are basically governed by the laws of the Quantum Mechanics. Nanotechnology involves these interdisciplinary knowledge areas and methodologies in order to study, manufacture and characterise functional structures with dimensions of tens of nanometers.

The NanoSpain network aims to agglutinate and coordinate the efforts made in the field of Nanotechnology by Spanish groups from universities, research institutes and companies. In addition, this network has tried to help the government institutions in defining potential actions and plans referring to this area. Currently, the network comprising 184 Spanish groups with near 1200 researchers in total is one of the widest Spanish scientific networks.

As a direct and most effective way to enhance interaction between the network members, two network meetings were organised in San Sebastian (2004) and Barcelona (2005) with respectively 210 and 260 participants registered. Due to this success, the network decided organising this year its third meeting in Pamplona with a similar format.

Its objective will also be to facilitate the dissemination of knowledge, promote interdisciplinary discussions among the different NanoSpain groups and enhance industrial participation. In order to organise the various sessions and to select contributions, the meeting will be structured in the following thematic lines, but interactions among them will be promoted:

1. Energy
2. NanoBiotechnology / Nanomedicine
3. NanoMaterials
4. NanoChemistry
5. NanoElectronics / Molecular Electronics
6. Nanomagnetism
7. Nanotubes
8. NEMS / MEMS
9. Scanning Probe Microscopies (SPM)
10. Scientific Policy
11. Simulation at the nanoscale

Working Groups (WG) will also be organised to enhance information flow between network partners and in particular:

- Exchange information of current work in specific research areas
- Solve particular technological problems
- Look for areas of common ground between different technologies
- Provide contributions to specific reports

The following WG will be organised:

1. Molecular Electronics (Coordinators: Julio Gómez & Pablo Ordejon)
2. NanoBiotechnology (Coordinator: Josep Samitier & Laura Lechuga)
3. NanoEnergy (Coordinators: Juan Roman Morante & Xavier Obradors)
4. NanoFabrication (Coordinators: Francesc Pérez-Murano & Fernando Briones)
5. Industrial (Coordinators: Isabel Obieta & Emilio Prieto)
6. NanoChemistry (Coordinators: Jaume Veciana & David Amabilino)

Another objective of this meeting will be to evaluate the situation of Nanotechnology in Spain, as well as reaching conclusions concerning the future of the NanoSpain network, in order to guarantee its continuity by means of concrete proposals.

In addition, thanks must be directed to the staff of all the organising institutions whose hard work has helped the smooth organisation and planning of this conference.

THE ORGANISING COMMITTEE

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Enrique Sahagún	Universidad Autónoma de Madrid

* Contact person: Antonio Correia – antonio@phantomsnet.net

KEYNOTES

Last Name	Name	Organisation	Country	Topic
Bourgoin	J.-P.	CEA Saclay	France	Nanotubes
Title: " <i>Self-assembling carbon nanotubes for electronics</i> "				
Brandbydge	Mads	Technical University of Denmark - MIC	Denmark	Molecular Electronics / Theory
Title: " <i>Electron-vibration interaction in atomic-scale conductors: inelastic transport and heating</i> "				
Fiorani	Dino	CNR	Italy	Nanomagnetism
Title: " <i>Nanomagnets for high density magnetorecording</i> "				
Hirscher	Michael	Max-Planck-Institut fuer Metallforschung	Germany	Energy
Title: " <i>Nanostructures with high surface area for hydrogen storage</i> "				
Kristensen	Anders	Technical University of Denmark - MIC	Denmark	NEMS/MEMS
Title: " <i>Lab-on-a-chip lasers</i> "				
Lorente	Nicolas	Universite Paul Sabatier	France	Theory
Title: " <i>Theory of electronic transport in the presence of vibrations on the atomic scale</i> "				
Pajot	Edith	INRA - Université Paris 11	France	Nanobiotechnology
Title: " <i>Nanobiosensors based on individual olfactory receptors</i> "				
Schift	Helmut	Paul Scherrer Institut	Switzerland	Nanofabrication
Title: " <i>Nanoimprint – A Versatile Patterning Technology</i> "				
Thompson	Carl V.	MIT	USA	Nanomaterials
Viviente	Jose Luis	EU - NMP	Belgium	Scientific Policy
Title: " <i>The European Union's 7th Framework Programme: NMP Priority</i> "				
Winterlin	Joost	Muenchen University	Germany	SPM
Title: " <i>Atomic processes on catalyst surfaces: many-body interactions and high pressure effects</i> "				

Exhibitors



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- Surface and material characterisation
- Vacuum and cryogenics instrumentation and technology
- Radiometry and photometry
- Particle counting

TELSTAR INSTRUMAT, S.L. counts amongst its customers the principal Official Organisation Investigation Centres and private customers in the microelectronic, aerospace, automotive, optical, food and pharmaceutical industries and in innovative fields such as biotechnology and nanofabrication. The company's head office is in Sant Cugat del Vallès (Barcelona) and it also has a branch office in Madrid.

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comercial@instrumat.telstar.es



BIOMETA was set up in 1998. Its activities are centred on the supply of products and services for research laboratories, industrial quality control and clinical diagnostic. The offices at Parque Tecnológico de Asturias centralize the main services: commercial department, warehouse and technical service. There is an spacious application laboratory where training courses take place quite often, as well as seminars and demos. In order to give the customer the best service there are commercial branches spreaded over the Spanish territory: Vigo, Bilbao, Barcelona, Valencia, Sevilla and Madrid, where the technical service is located as well. The current staff is formed by 21 people, most of them with a high degree and wide experience. Materials Science is one of the most relevant fields in which Biometa participates. The following are some of the most important companies represented by Biometa in Spain:

BUEHLER: Metallography / **GALDABINI:** Universal Testing Machine / **PSIA:** Atomic Force Microscopes **HYSITRON:** Nanoindenters / **LENTON:** Camera and Tube furnaces up to 1800°C **RETSCH:** Grinding of samples. Particle size analysis / **FLUXANA:** Sample preparation and accessories for XRF **SURFACE:** UHV-PLD projects and installations / **PARR:** Combustion calorimeters. Laboratory reactors

Biometa

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TECNOLOGÍA DE VACÍO S.L. was created in 1.996, with the main aim to represents in Spain and Portugal the European vacuum manufacturer leader Companies, such as PFEIFFER VACUUM and VAT. In 1.999 we started our activity in tribology, dealing with systems from CSM.

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If you would like to contact us, please send an e-mail to: info@sodena.com. If you would like to send queries, suggestions or get more information, please visit the queries and suggestions page.

SODENA

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The Agency of Innovation of Navarre is a public corporation founded in 1999 by the Government of Navarre. Our goal is to globally manage innovation in Navarre, using a coordinated and pragmatic approach. The Agency exercises the task of promoting an increase in innovation that is both qualitative and quantitative.

Among several other tasks the Agency has entrusted the execution of the Technological Plan of Navarre, whose objective it is to improve the quality of life of the citizens and to impel a policy of sustainable development of the society of Navarre. We will achieve this by actively bringing together the activities of I+D+I in companies, Technological Centers and Universities.

Mission statement

To serve the Historical Community of Navarre promoting

- 1) a qualitative and quantitative increase on innovation
- 2) an enhancement on the competitiveness of our companies
- 3) creation of employment
- 4) an improvement on services provided by the administration. With this approach the Agency intends to increase the well-being and the present and future quality of life in our society.

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3rd NANOSPAIN WORKSHOP: PROGRAMME

Sunday March 19, 2006	
19h00-20h00	Registration
20h30	Welcome Reception at Baluarte

SCIENTIFIC PROGRAMME	
Monday March 20, 2006	
08h00-09h00	Registration
09h00-09h10	Conference Opening
Chairman: Fernando Palacio	
09h10-10h00	Dino Fiorani (CNR, Italy) " <i>Nanomagnets for high density magnetorecording</i> "
10h00-10h20	Javier Tejada (Universidad de Barcelona, Spain) " <i>Teaching quantum nanomagnetism</i> "
10h20-10h40	Marisol Martin-Gonzalez (IMM-CSIC, Spain) " <i>Interfacial magnetism in ZnO/MnO₂ and ZnO/Co₂O₃ thin films and multilayers</i> "
10h40-11h00	T. Cristina Rojas Ruiz (ICMSE-CSIC, Spain) " <i>Microstructure and Magnetic behaviour of alkanethiol-capped gold nanoparticles</i> "
11h00-11h40	Coffee Break / Poster Session & Exhibition
Chairman: Juan Jose Saenz	
11h40-11h45	Juan Jose Saenz (Universidad Autonoma de Madrid, Spain) " <i>M4Nano Initiative</i> "
11h45-12h35	Nicolas Lorente (University Paul Sabatier, France) " <i>Theory of electronic transport in the presence of vibrations on the atomic scale.</i> "
12h35-12h55	Daniel Sanchez Portal (DIPC, CSIC-UPV/EHU, Spain) " <i>Resonant charge transfer at surfaces: an ab initio approach</i> "
12h55-13h15	Eduardo Machado (Instituto de Ciencias de Materiales de Barcelona-CSIC, Spain) " <i>First-principles Simulations of the Charge Density Waves STM Images of Quasi-one-dimensional Materials</i> "
Lunch	
Chairman: Jaume Veciana	
15h20-15h40	Imma Ratera (Instituto de Ciencias de Materiales de Barcelona-CSIC, Spain) " <i>Charge Transport Properties of Donor-Acceptor Organic Radicals and Self Assembled Organic Monolayers</i> "
15h40-16h00	Abderrazzak Douhal (UCLM-Laboratorio de Fisica Química, Spain) " <i>Ultrafast Dynamics of CdTe Nanoparticles in Water Solution</i> "
16h00-17h00	Flash Contributions (Topics: Nanomagnetism, Nanochemistry, Nanoelectronics, NEMS/MEMS, Energy)
17h00-20h00	Poster Session / Coffee Break
20h00	Reception at Baluarte

SCIENTIFIC PROGRAMME

Tuesday March 21, 2006

Chairman: Jesus Perez Conde		
09h10-09h30	Wolfgang Maser (Nanozar S.L., Spain) " <i>Carbon Nanotubes: Towards technological applications</i> "	
09h30-10h20	Michael Hirscher (Max-Planck-Institut fuer Metallforschung, Germany) " <i>Nanostructures with high surface area for hydrogen storage</i> "	
10h20-11h20	Coffee Break / Poster Session & Exhibition	
Chairman: Wolfgang Maser		
11h20-11h40	Jose M. Abad-Pastor (University of Liverpool, UK) " <i>Synthesis of silver nanoparticles with great monodispersity and long-term stability in aqueous solution</i> "	
11h40-12h00	Albert Romano-Rodriguez (Universidad de Barcelona, Spain) " <i>AC Impedance Spectroscopy of individual tin-oxide contacted using Dual Beam FIB nanolithography</i> "	
12h00-12h50	Carl V. Thompson (MIT, USA) " <i>Templated Self Assembly for Organization of Systems of Nanomaterials</i> "	
12h50-14h50	Lunch	
Chairman: Fernando Briones		
14h50-15h10	Manuel Vazquez (MEC, Spain) " <i>Spanish Nanotechnology Programme</i> "	
15h10-15h30	Flash Contributions: MEC funded projects (3)	
	Ricardo Ibarra (Instituto de Nanociencia de Aragón, Spain)	
	Rafael Moliner (Instituto de Carboquímica-CSIC, Spain)	
	Florencio Sanchez (ICMAB-CSIC, Spain)	
15h30-15h40	Fernando Beltran (Gobierno de Aragón, Spain)	
15h40-16h00	Jose-Luis Viviente (EU-NMP, Brussels) " <i>The European Union's 7th Framework Programme: NMP Priority</i> "	
16h00-16h15	Jesus Zabalo (SODENA, Spain)	
16h15-16h30	Laura Lechuga (IMM -CSIC, Spain) " <i>Nanomedicine Platform</i> "	
16h30-16h45	David Mecerreyes (CIDETEC, Spain) " <i>Nanoelectronics Platform</i> "	
16h45-17h00	Jaume Veciana (ICMAB - CSIC, Spain) " <i>Nanochemistry Platform</i> "	
17h00-17h30	Coffee Break / Poster Session & Exhibition	
17h30-20h00	<i>Working Groups (parallel sessions)</i>	
	Molecular Electronics	
	Nanofabrication F. Perez Murano (CNM, Spain)	
	Nanobiotechnology	
Nanoenergy	17h30-17h45	Javier Sanchez (Carbueros Metalicos/MATGAS, Spain)
	17h45-18h00	Oscar Miguel (CIDETEC, Spain)
	18h00-18h15	M. P. Pina (Universidad de Zaragoza, Spain)
	18h15-18h30	J.R. Morante (UB/CeRMAE, Spain)
	18h30-18h45	Xavier Obradors (ICMAB/CeRMAE, Spain)
	18h45-20h00	Discussion
Industrial	17h30-17h45	Isabel Obieta (Inasmet, Spain) " <i>Nanomaterials: Opportunities and Challenges</i> "
	17h45-18h00	Javier García (Aenor, Spain) " <i>Nanotechnologies Standardisation</i> "
	18h00-18h15	Cesar Merino (Grupo Antolin, Spain) " <i>Structural and Surface Characterization of Ni-derived Carbon Nanofibers by Floating Catalyst Method</i> "
	18h15-18h30	Eugenio Vilanova (Universidad Miguel Hernandez de Elche, Spain) " <i>The usual strategy to evaluate safety of chemicals can be applied to products developed under nanoscience or nanotechnology?</i> "
	18h30-18h45	Emilio Prieto (CEM, Spain) " <i>Quantitative nanotechnology – the role of nanometrology</i> "
	18h45-19h00	Carles Escolano (Willems & van den Wildenberg, Spain) " <i>Nanomaterials Roadmap</i> "
	19h00-19h15	Rafael Muguerza Eraso (Gobierno de Navarra, Spain)
	19h15-20h00	Discussion

	Nanochemistry	17h30-17h45	Jose C. Conesa (ICP-CSIC, Spain)
		17h45-18h00	Carmen Ocal (ICMM-CSIC, Spain)
		18h00-18h15	Jose Luis Serrano (INA, Spain)
		18h15-18h30	Conxita Solans (IIQAB-CSIC, Spain)
		18h30-20h00	Discussion
21h30	<i>Conference Dinner (Restaurant: Palacio Castillo de Gorraiz)</i>		

SCIENTIFIC PROGRAMME
Wednesday March 22, 2006

Chairman: Javier Mendez

09h00-09h50	Joost Wintterlin (Muenchen University, Germany) " <i>Atomic processes on catalyst surfaces: many-body interactions and high pressure effects</i> "
09h50-10h10	Jorge Iribas Cerda (ICMM-CSIC, Spain) " <i>Subsurface structure of epitaxial silicides imaged by STM</i> "
10h10-10h30	Jordi Toset (PCB - Universidad de Barcelona, Spain) " <i>Electrostatic manipulation of gold nanoparticles using an atomic force microscope</i> "

10h30-11h30 **Coffee Break / Poster Session & Exhibition**

Chairman: Pablo Ordejon

11h30-12h20	Jean-Philippe Bourgoin (CEA Saclay, France) " <i>Self-assembling carbon nanotubes for electronics</i> "
12h20-12h40	Teresa de los Arcos (UNIBAS, Switzerland) " <i>Understanding carbon nanotube growth with photoelectron spectroscopy</i> "
12h40-13h00	Fernando Langa (UCLM, Spain) " <i>New methods of functionalization of Single-Wall Carbon Nanotubes</i> "

13h00-15h00 **Lunch**

Chairman: Juan Manuel Irache

15h00-15h50	Edith Pajot (INRA- Universite Paris 11, France) " <i>Nanobiosensors based on individual olfactory receptors</i> "
15h50-16h10	Javier Tamayo (IMM-CSIC, Spain) " <i>Development of Nanomechanical Biochips for Functional Genomics and Proteomics</i> "
16h10-16h30	Jose A. Martin Gago (ICMM-CSIC, Spain) " <i>Self-assembled monolayers of peptide nucleic acids: from the molecular structure to biosensor applications</i> "
16h30-16h50	Jesús M. De la Fuente (CICIC-CSIC, Spain) " <i>Water Soluble Magnetic Glyconanoparticles: Synthesis, Characterization, Cell response and Applications as Contrast Agents for MRI</i> "
16h50-17h50	Flash Contributions Topics: (Nanobiotechnology/Nanomedicine, Nanotubes, Nanomaterials)

17h50-20h00 **Poster Session / Coffee Break**

SCIENTIFIC PROGRAMME**Thursday March 23, 2006****Chairman: Daniel Sanchez Portal**

09h00-09h50	Mads Brandbydge (MIC, Denmark) " <i>Electron-vibration interaction in atomic-scale conductors: inelastic transport and heating</i> "
09h50-10h10	Nicolas Agrait (Universidad Autónoma de Madrid, Spain) " <i>Mechanical properties of suspended atomic chains of gold</i> "
10h10-10h30	Benito Alen (IMM-CSIC, Spain) " <i>High resolution optical spectroscopy of single self-assembled quantum dots and rings</i> "

10h30-11h00

Coffee Break**Chairman: Emilio Prieto**

11h00-11h50	Helmut Schiff (Paul Scherrer Institut, Switzerland) " <i>Nanoimprint – A Versatile Patterning Technology</i> "
11h50-12h10	Nuria Barniol (Universidad Autónoma de Barcelona, Spain) " <i>Nanoresonators with integrated circuitry for high sensitivity and high spatial resolution mass detection</i> "
12h10-12h30	Rodrigo Fernandez Pacheco (Institute of Nanoscience of Aragon (INA) - UNIZAR, Spain) " <i>Synthesis of magnetic nanostructured silica-based materials as possible vectors for drug-delivery applications</i> "
12h30-12h50	Jordi Esquena (Instituto de Ciencias Ambientales-CSIC, Spain) " <i>Preparation of mesoporous silica with small pore size and thick walls, by using fluorinated surfactants</i> "
12h50-13h40	Anders Kristensen (Technical University of Denmark, Denmark) " <i>Lab-on-a-chip lasers</i> "
13h40-14h00	"3rd NanoSpain Workshop & WG" Conclusion Remarks Closing

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Pamplona 20-23, March 2006



3rd NANOSPAIN WORKSHOP

ABSTRACTS

Pamplona 20-23, March 2006



3rd NANOSPAIN WORKSHOP

KEYNOTE CONTRIBUTIONS

SELF-ASSEMBLING CARBON NANOTUBES FOR ELECTRONICS

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During the last five years, Carbon Nanotubes have been shown to be very promising building blocks for nanoelectronics. Indeed, they exist as semiconducting or metallic wires and have been used to fabricate nm-scale devices like transistors, diodes, NEMs or SET (single electron transistor) for example. The future of SWNT-based devices in nanoelectronics is to a large extent related to the development of bottom-up self-assembly techniques. In this talk, the focus will be on the self-assembled nanotube devices that were developed recently at the LEM.

I will show how carbon nanotubes(NTs) can be self-assembled at predefined location of a substrate using a localized functionalization of the substrate by a patterned self-assembled monolayer^{1,2}. Three examples of application of that technique to the realization of devices will be presented:

- ◆ Field effect transistors devices prepared in that way prove functional with state-of-the-art performances^{3,4}. Their high frequency (GHz) behaviour was investigated and a high frequency equivalent circuit was derived for the first time⁵. The role played by the environment (including that of the self-assembled monolayer directing the deposition of the NTs and that of molecules adsorbed on the NTs) on the CNTFET devices characteristics will also be discussed. It will be shown in particular how a chemical treatment of the devices can be used to drastically improve the performances of the CNTFET^{3,4}.
- ◆ Further elaborating upon the chemical tailoring of the self-assembled CNTFET devices, a new class of devices consisting of optically gated CNTFET or memories has been developed and will be presented⁶.
- ◆ New nano electromechanical systems(NEMS) based on nanotubes can also be self-assembled with that technique, that function as very efficient switches with the current changing by several orders of magnitude within a 100mV change of the actuating electrode bias⁷. Nanotubes are indeed quite promising as core elements of NEMS. Clearly, the development of such NEMS requires understanding the interplay between the physical, geometrical and electrical parameters of the system. I will show that these parameters and the deflection efficiency of MWNTs are related through a scaling law of general validity that can be used as an efficient dimensioning tool for nanotube NEMS⁸.

Finally, the improvements of the self-assembling technique using the recognition properties of biomolecules will be presented⁹.

With the collaboration of:

S. Auvray, J. Borghetti, V. Derycke, M.F. Goffman, P. Chenevier, L. Goux-Capes, A. Filoramo, R. Lefevre, S. Streif, K. Nguyen, S. Lyonnais, LEM ; J. M. Bethoux, H. Happy, G. Dambrine, S. Lenfant, D. Vuillaume (IEMN Lille); P. Hesto (IEF Orsay) and L. Forro (EPFL Lausanne)

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ELECTRON-VIBRATION INTERACTION IN ATOMIC-SCALE CONDUCTORS: INELASTIC TRANSPORT AND HEATING

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In molecular electronics the inelastic scattering of traversing electrons and energy dissipation play essential roles for device characteristics, working conditions, and stability. The signatures of interactions with vibrations can be observed in the current-voltage characteristics of atomic-scale conductors. These vibrational signals may be used to extract information about the detailed atomic configuration – information usually not accessible simultaneously with transport measurements.

In this talk we discuss theoretical work on inelastic transport due to interaction with atomic vibrations in atomic-scale conductors, which are strongly coupled to electrodes. Here we focus primarily on atomic wire systems [1], where the calculated inelastic signals can be directly compared to detailed experiments, see Fig. 1. We present extensive calculations on gold atomic wires/chains with different lengths and strain, and present preliminary results for platinum wires. The case of molecular contacts will also be touched upon.

Our results are obtained using parameter-free calculations based on density functional theory combined with non-equilibrium Greens functions (NEGF) [2]. The inelastic effects are taken into account using the self-consistent Born approximation (SCBA) [3]. While the full NEGF-SCBA calculations are rather computationally demanding, we show how these equations can be simplified in a lowest order expansion (LOE). The LOE yield excellent agreement with our full SCBA results and may be justified in many cases [4]. We can obtain simple analytical formulas which we demonstrate can be used to fit experimental data to extract various parameters, e.g. the electron-hole damping rate. We can calculate the power transferred to the vibrations and the damping of the vibrations due to electron-hole pair excitation. This enables us to determine an upper bound on the vibrational excitation in the conductor.

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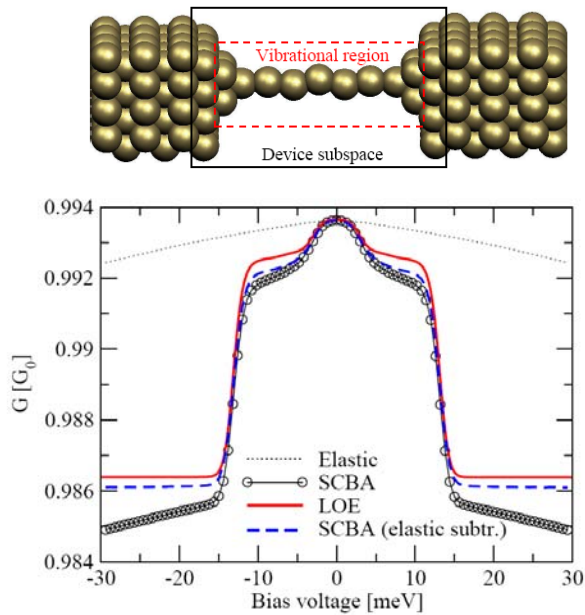
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Fig. 1: Calculation of the inelastic signal in conductance vs. bias voltage in a 7-atom long gold chain connected to gold electrodes. We show how these signals are related to the atomic geometry of the chain (e.g. length and strain).

NANOMAGNETS FOR HIGH DENSITY MAGNETORECORDING

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Magnetic materials engineered at the nanometer scale (thin films, multilayers, nanoparticles, nanocomposites, nanowires) exhibit novel physical properties and phenomena, which are opening new frontiers in fundamental research and technological applications. The size confinement to the nanometer scale induces significant changes in the magnetic properties, as some important characteristic physical lengths, e.g. the exchange correlation length and the thickness of the domain wall, are on nanometer scale.

Magnetic nanoparticles have been the object of intense investigations, since the end of 40's (Néel theory) for both fundamental (they represent model systems for investigating magnetization reversal mechanisms) and applications (in geology, biology, medicine, catalysis, archaeology, magnetorecording, sensors...) point of view.

Current conventional magnetic media for hard disks consist of nanogranular continuous films with the magnetization aligned along the plane of the disk (longitudinal magnetorecording). Each bit consists of a collection of a large number of grains to statistically reduce the noise. The latest commercial disks achieve densities of 100 Gbit/in². Higher densities would require smaller and smaller bits, with smaller and smaller particles. However, when these particles become so small that their magnetic anisotropy energy (proportional to the particle volume) becomes comparable to the thermal energy, they can become unstable, i.e. their moment can flip spontaneously, and then their information content is lost. Since the current technology has already reached its physical limits, a radically different solution, with a completely different architecture of the magnetic media, is necessary for a significant progress beyond the current recording density.

Among the alternative technologies, one of the most promising is represented by the patterned media with the magnetic moments perpendicular to the surface of the disk (perpendicular magnetorecording). They consist of regular arrays of single domain nanomagnets separated by a non magnetic matrix.

The HIDEMAR european project, lead by ISM/CNR, was successful in realizing a patterned prototype hard disk with a density of 208 Gbit/in². Co/Pd multilayers, with high perpendicular anisotropy, were deposited onto disks by sputtering under industrial conditions and were patterned using electron beam lithography. The patterned media consisted of circular tracks of magnetic dots measuring just 27 nm in diameter, with a periodicity of 60 nm.

NANOSTRUCTURES WITH HIGH SURFACE AREA FOR HYDROGEN STORAGE

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The major bottleneck for commercializing fuel-cell vehicles is onboard hydrogen storage. The presently available systems are high pressure tanks or liquefied hydrogen in cryogenic vessels, which both possess severe disadvantages. Storage in light-weight solids could be the solution to this problem. Two principle storage mechanisms exist: i) Adsorption of hydrogen molecules on surfaces, i.e., physisorption. ii) Hydrogen atoms dissolved or forming chemical bonds, i.e., chemisorption.

The presentation will focus on physisorption of hydrogen on new nanoscale materials with high specific surface area. These microporous materials show a high potential for hydrogen storage at lower temperatures. Carbon nanomaterials possess high specific surface area, microporosity, and low mass. Apart from these characteristics, materials like activated carbons are cheap and easy to produce. It can be shown for different carbon nanomaterials that the storage capacity depends linearly on the BET specific surface area (SSA), see Fig.1, and is independent of the individual nanostructure [1-3]. Zeolites are aluminosilicates with a very open microporous structure with channels that are large enough to contain gas molecules. Moreover, the presence of electrostatic forces within the channels is a unique characteristic of the zeolites. For zeolites a similar relation between the storage capacity at low temperatures and the SSA is found [4], however, the SSAs obtained for zeolites are typically smaller. In recent years a new class of materials with high specific surface area, the metal-organic frameworks (MOFs), have been developed and studied for gas adsorption [5,6]. These MOFs consist of metal oxide clusters connected by rigid aromatic linkers giving a three dimensional porous structure and, furthermore, they possess the lowest density of all known crystalline materials. Newest measurements on the hydrogen uptake in MOFs will be discussed, e.g. [7-10]. As for other microporous adsorbents, for MOFs an almost linear correlation between the maximum hydrogen uptake and the SSA has been found [10], see Fig. 2. Together these results indicate that nanostructures with high SSA and micropore density are very promising materials for hydrogen storage at low temperature which, e.g., may be used for cryogenic storage systems in long-term satellite missions.

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Figures:

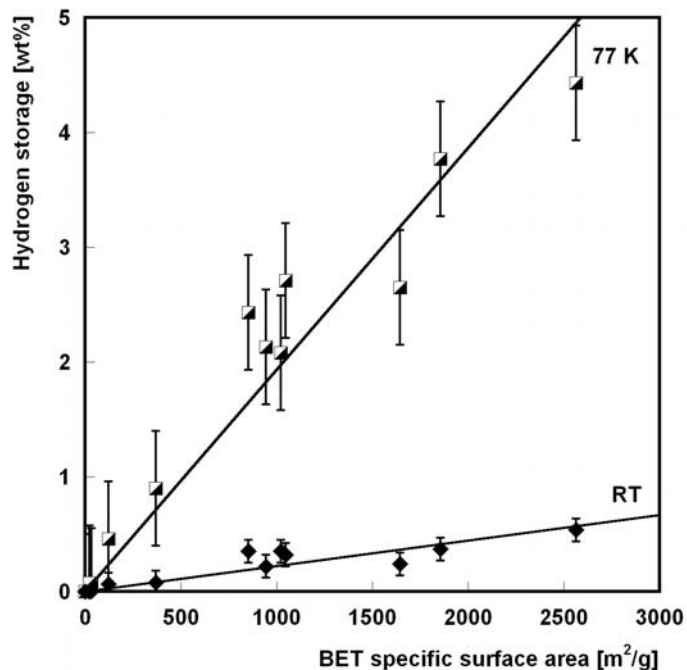


Fig. 1: Hydrogen storage capacity of various carbon nanostructures versus the BET specific surface area at 77 K and RT, as published in [3].

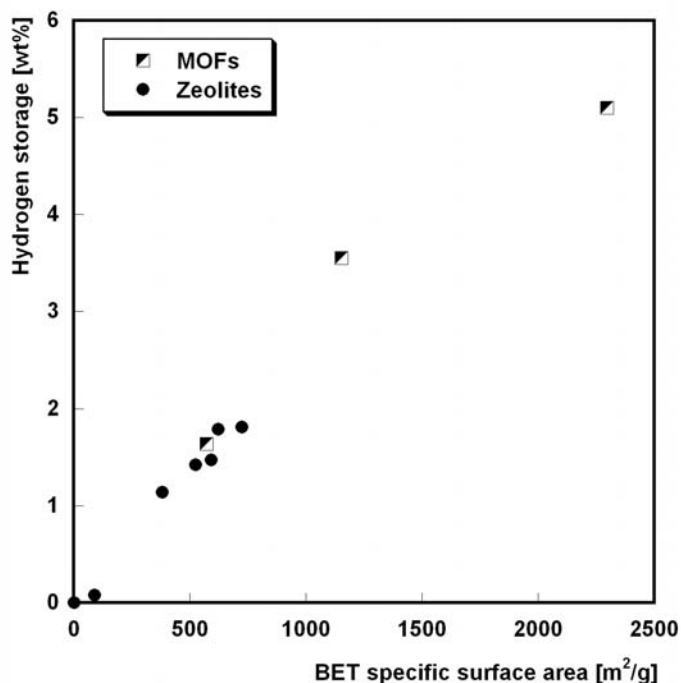


Fig. 2: Hydrogen storage capacity corresponding to the saturation value at 77 K as a function of the BET specific surface area for crystalline microporous materials, metal-organic frameworks MOFs [7,10] (squares) and zeolites [4] (dots), as published in [10].

LAB-ON-A-CHIP LASERS

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Light sources that can be integrated onto lab-on-a-chip micro-systems are of high interest for on-chip spectral analysis of chemical samples [1]. For these applications dye lasers are of particular interest due to the possibility of tuning the wavelength in the visible range. Such applications have stimulated an increasing effort in realizing chip based dye lasers by glass or polymer microfabrication [2-10].

We present a technology for miniaturized, polymer based lasers, suitable for integration with planar waveguides and microfluidic networks. The lasers rely on the commercial laser dye Rhodamine 6G as active medium, and the laser resonator is defined in a thin film of polymer on a low refractive index substrate. Two types of devices are demonstrated: microfluidic- and solid polymer dye lasers. In the microfluidic dye lasers [2-8], the laser dye is dissolved in a suitable solvent and flushed through a microfluidic channel, which has the laser resonator embedded. For solid state dye lasers [9-10], the laser dye is dissolved in the polymer forming the laser resonator. The miniaturized dye lasers are optically pumped by a frequency doubled, pulsed Nd:YAG laser (at 532 nm), and emit at wavelengths between 560 nm and 590 nm. The lasers emit in the plane of the chip, and the emitted light is coupled into planar polymer waveguides on the chip. The feasibility of three types of polymers is demonstrated: SU-8, PMMA and a cyclo-olefin co-polymer (COC) - Topas. SU-8 is a negative tone photoresist, allowing patterning with conventional UV- [9,10] or e-beam lithography [11]. PMMA and Topas are thermoplasts, which are patterned by nanoimprint lithography (NIL)[12,13]. The lasing wavelength of the microfluidic dye lasers can be coarse tuned over 30 nm by varying the concentration of laser dye, and fine tuned by varying the refractive index of the solvent. This is utilized to realize a tunable laser, by on-chip mixing of dye, and two solvents of different index of refraction [8]. The lasers were also integrated with waveguides and microfluidic networks [14].

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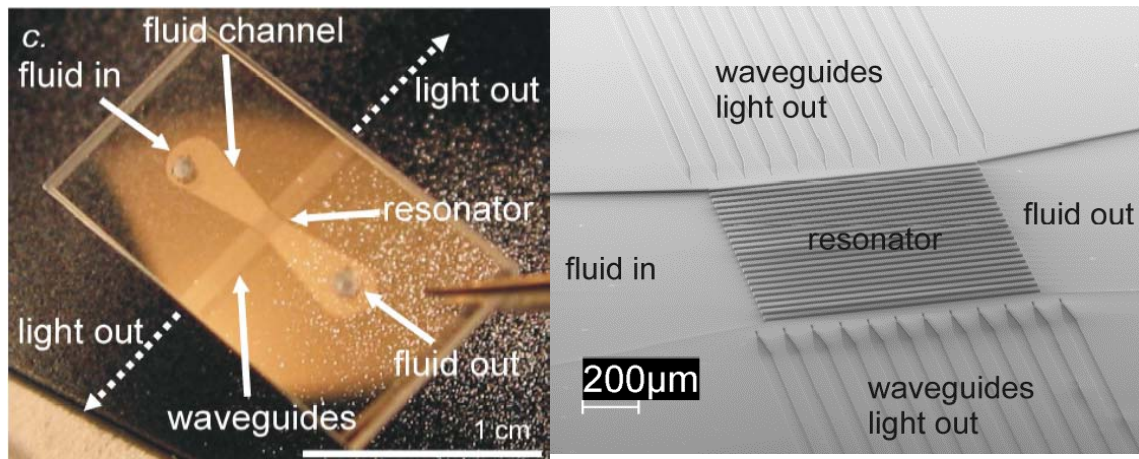


Fig. 1 Microfluidic dye laser. The microfluidic channel with embedded optical resonator is defined in a single lithography step in a 10 mm thick polymer film, sandwiched between two glass substrates. The laterally emitting DFB laser resonator is formed by polymer walls embedded in the microfluidic channel.

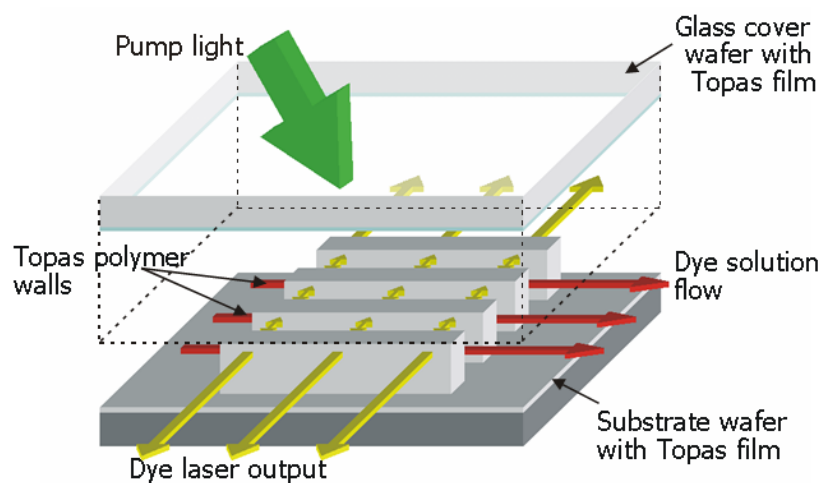


Fig. 2 Outline of the laterally emitting microfluidic dye laser resonator.

THEORY OF ELECTRONIC TRANSPORT IN THE PRESENCE OF VIBRATIONS ON THE ATOMIC SCALE.

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In this talk, I will present electron-current induced dynamics in condensed matter systems in the low-conductance and high-conductance regimes. The low-conductance case deals with the inelastic effects induced in tunnelling junctions. The properties of tunnelling currents allow for unique control capabilities. Indeed, I will make a brief summary of the achievements and understanding attained in the spectroscopic analysis of vibrations induced on adsorbates on metallic surfaces with a scanning tunnelling microscope (STM) [1]. I will show that the simulation of inelastic electron tunnelling spectra is needed for determining the excited modes and identifying the measured species. Recently, we have been able to determine the product of an STM-induced reaction on benzene by simulating the spectra of the different possible products [2].

The ability to excite specific vibrations permits to select atomic dynamics by pumping energy in given reaction coordinates. Hence, the STM parameters can be tuned to drive one type of mode above a specific dynamical barrier. In this way, the redistribution of energy from the excited mode to the different molecular degrees of freedom permits overcoming this barrier. On the other hand, repeated excitation of another mode can lead to overcoming a second barrier along a different reaction pathway. I will show recent experimental and theoretical data about mode selective dynamics on ammonia molecules chemisorbed on Cu(100) [3].

The high-conductance case corresponds to the ballistic regime. The electron current is not a tunnelling current, and the mean free path of electrons is much larger than the typical dimensions of the atomic objects. Recent experimental data have shown that it is possible to excite localized vibrations in monoatomic gold chains in this regime [4] akin to vibrational spectroscopy in the tunnelling regime. I will briefly review recent theoretical work [5] that reveals the modes excited by the ballistic current, as well as the difference between the heating of atomic wires and the dynamics induced on molecules by the STM.

Vibrations can eventually create electronic currents. This is the case of dangling-bond vibrations in a semiconducting surface. Indeed, the otherwise "state-in-the-gap" that is a dangling bond on a Si(111) $\sqrt{3}\times\sqrt{3}R30^\circ$ -B surface, can become connected with the acceptor (boron, B) band via its large electron-vibration coupling, Figure 1. The role of the vibration is to permit the electron flow between the tip of an STM and the bulk boron band [5]. Due to the long lifetimes and large couplings involved in this process, the need of an all order theory is mandatory and new theoretical schemes are presented.

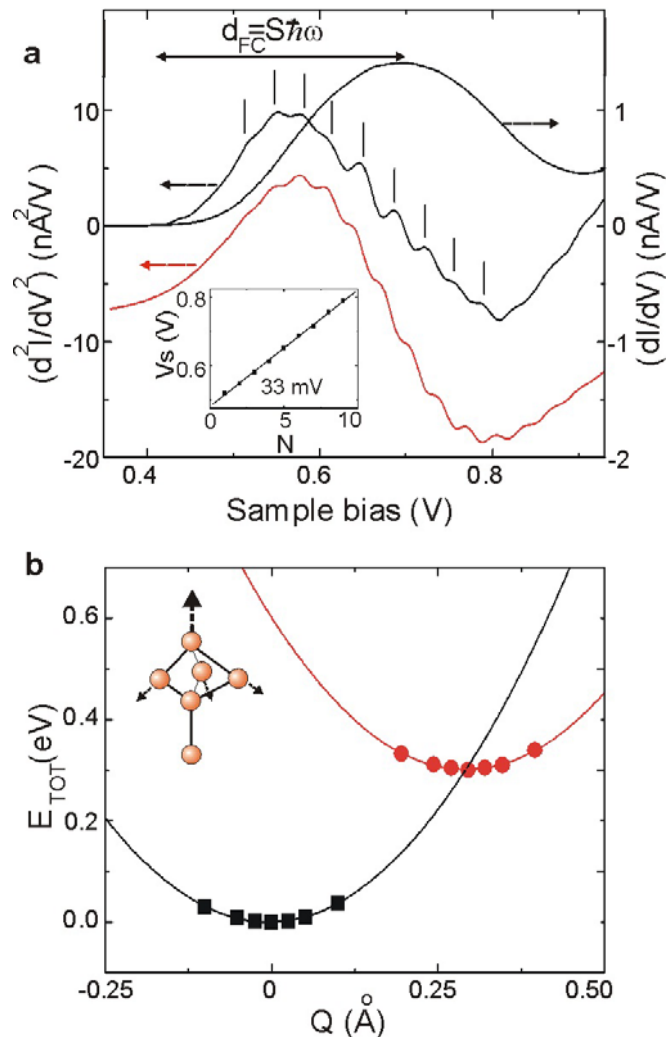


Figure 1 Vibronic states of an isolated Si dangling bond on a Si(111)- $\sqrt{3}\times\sqrt{3}$ R30°-B surface. **a**, Experimental (black) and calculated (red) d^2I/dV^2 spectra, shifted for clarity and obtained on a bright adatom. The vertical lines indicate the position of equally spaced peaks in the spectrum. The Franck Condon shift $d_{FC} = S\hbar\omega$ is deduced from the width at half maximum of the dI/dV peak. The curves were acquired with feedback parameters $V_{sample} = +1.5$ V and $I = 500$ pA at 5 K. Inset : Plot of the peak energy versus the peak number N for the vibronic progression, yielding the energy of the vibrational mode. **b**, Total energy of a neutral (black) and a negative charge (red) adatoms, calculated by density functional theory, versus the lattice coordinate Q of the adatom. The fit of the plots shows a harmonic behaviour and yields a quantum of vibration of 32.5 meV for the stretching mode.

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Nanobiosensors based on individual olfactory receptors

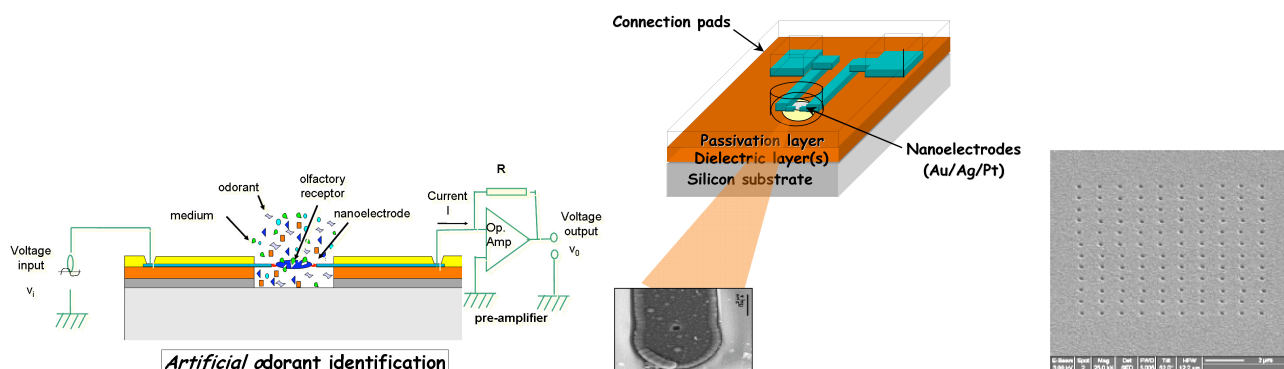
Edith Pajot-Augy

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Animals such as rats, dogs, but also bees, can detect Volatile Organic Compounds specifically and with very low thresholds, which is used in fields as various as explosives or drugs detection, and also for medical diagnosis in cases where VOCs are associated to a given pathology. Presently, electronic noses are based on the detection and discrimination of complex odorant mixtures via a network of sensors with a broad spectrum, that generate a characteristic response pattern. Comparing this profile to a database of patterns generated by standards allows the identification and qualification of the odorants present in the mixture. These chemical sensors rely on various physical techniques (electrical, optical, calorimetric, gravimetric, ...) to estimate parameters able to discriminate the odorants present. However, if those sensors display some sensitivity and capacity to analyze odorant mixtures, objectivity, and rapidity, they are nevertheless limited in terms of specificity, stability, and hampered by the presence of water, ... Electronic noses are presently developed and miniaturized at the level of micro e-noses. Meanwhile, a number of cell-based biosensors have been designed, using yeasts, or more specialized taste or olfactory sensory neurons, or even cells recombinantly expressing olfactory receptors, so as to measure changes of electrical parameters in the presence of odorants.

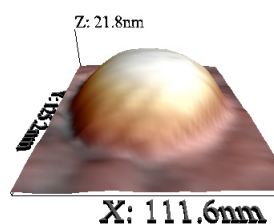
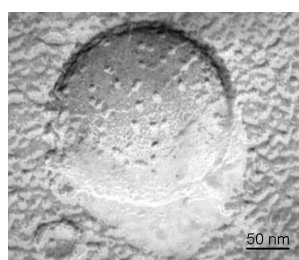
A further step is to use the olfactory receptors themselves as a source of sensing elements for biosensors, using various methods such as BioFETs, SPR, piezoelectricity, or 2nd messengers, to monitor their functional response to odorants. Such sensors benefit the natural biological optimization of the molecular recognition of an odorant by its receptor, which ensures the response specificity and reproductibility. They give a potential access to all kinds of odorants, with the very low detection thresholds observed on the animals ($10^{-9}M$... $10^{-12}M$... $10^{-14}M$), and they can work in an aqueous environment, contrary to chemical sensors. However, since receptors are expressed in low amounts in olfactory sensory neurons, and several hundred different receptors are expressed each in another neuron, the primary requirement is that of an adequate expression system for olfactory receptors. The yeast *S. cerevisiae* proved efficient to reach a quantitative functional expression and adequate trafficking of olfactory receptors to the plasmic membrane under optimized induction conditions.

The purpose of the European project "SPOT-NOSED" (<http://www.nanobiolab.pcb.uv.es/projectes/spotnosed/>) was the development of a nanobiosensor array based on the electrical properties of single olfactory receptors, to mimic the performances of natural olfactory sensing system.

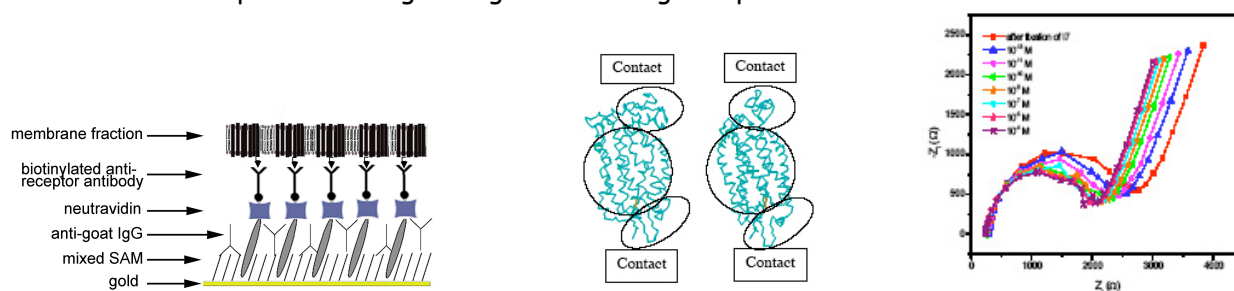


The nanobiosensor array will integrate nanotransducers consisting of gold nanoelectrodes with a "single" olfactory receptor anchored in it. In the framework of this project, an OR and an

appropriate G_{α} protein were co-expressed in yeast cells from which membrane nanosomes, with size homogenized to around 50 nm by sample sonication, were prepared.

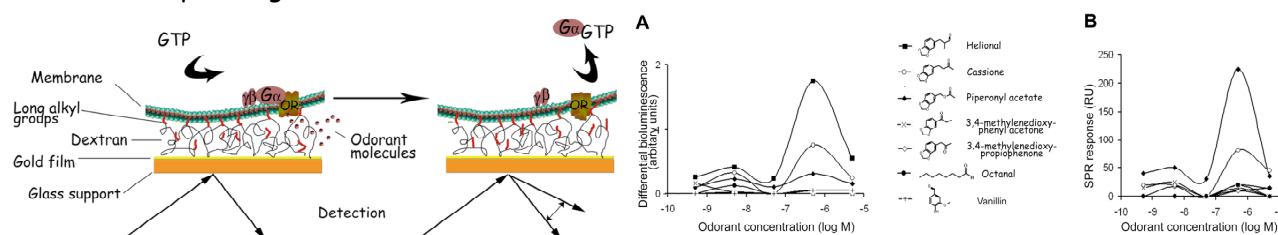


A gold surface was sequentially functionalized with mixed Self Assembled Monolayers providing a controlled density of anchoring sites, neutravidin, and specific biotinylated receptor antibody. Electrochemical Impedancemetric Spectroscopy was performed at each step, and significant changes were also detected upon the final grafting of increasing receptor amounts.



The nanovesicles containing functional olfactory receptors are grafted onto functionalized substrates without disruption, and provide a high surface coverage, as visualized by means of Atomic Force Microscopy. Impedancemetric detection of the individual olfactory receptors conformational change upon odorant ligand binding is expected to endow these sensors with a far better specificity, detection threshold, reproducibility, and odor spectrum than traditional physical sensors.

In parallel to EIS, Surface Plasmon Resonance performed on the same nanosomes grafted on a sensorchip allowed to quantitatively evaluate OR stimulation by an odorant, and G protein activation. This demonstrates that ORs in isolated nanosomes immobilized on sensorchips retain their full activity and discriminate between odorant ligand and unrelated odorants, as previously shown in whole yeast cells with a reporter gene.



These findings will allow the development of a new generation of nanosensors, bioelectronic olfaction devices for rapid and noninvasive assessment of VOCs, that can constitute a signature of metabolic states or diseases, participate in aromas in food, be associated with drugs and explosives or to domestic and environmental pollutants. Ligand screening for orphan receptors and pharmacological screening may constitute further high value applications.

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NANOIMPRINT – A VERSATILE PATTERNING TECHNOLOGY

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Since nanoimprint lithography (NIL) has emerged as an alternative nanopatterning technology in 1995, many groups around the world have joined the NIL Community. The impressive sub-10nm resolution capability of thermoplastic molding, went far ahead of what current high end lithographic technologies are providing. And while the resolution issue alone proposed NIL as a serious Next Generation Lithography candidate, the straight forward and low-cost process is promising to a lot of other applications.

NIL was first reported as thermoplastic molding [1], and is therefore often referred to as hot embossing lithography (HEL) [2]. The unique advantage of a thermoplastic material is that the viscosity can be changed to a large extent by simply varying the temperature [3]. Thermoplastic molding is known since long, and many materials are available with a range of physical, optical, and chemical properties, which makes it possible to it for applications ranging from integrated optics, microfluidics to liquid crystal displays [4,5]. Apart from this, process variations using UV curable materials and hybrid approaches are developed.

PSI, which over the years had gained a strong expertise in fabricating nanostructured optical elements by different molding techniques, started its nanoimprint activity quite early [2]. Nanoreplication techniques were used for several applied projects, partly with industrial contribution. PSI is also participating in the European Integrated Project **NaPa**, which is an effort to bring together expertise and manpower on Emerging Nanopatterning Technologies within Europe. Within NaPa, aspects of NIL ranging from materials, tools, stamps, process development and applications, including industrial demonstrators, are investigated.

In my presentation I will give an overview about current developments, and not only show applications of replication for resist patterning, but also broaden the view for applications in the non-lithographic area, including roll embossing of textile fibers.

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TEMPLATED SELF ASSEMBLY FOR ORGANIZATION OF SYSTEMS OF NANOMATERIALS

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Materials in the form of nano-scale dots, wires, and tubes have remarkable properties that suggest break-through applications in electrical, photonic, electromechanical, and magnetic micro- and nano-systems. However, to integrate nano-materials into such systems requires new approaches to their placement in complex two- and three-dimensional arrays. For large and complex systems, placement must be accomplished in parallel processes, in which large numbers of nano-materials or structures are formed simultaneously. There are two basic placement strategies (schematically illustrated in Figure 1); growth or formation of nanomaterials in the final desired locations (grow-in-place) or growth or formation of nanomaterials in separate processes, followed by placement in the locations for system integration (grow-then-place) [1]. Both approaches require patterned *placement cues*, such as catalysts for grow-in-place approaches or topographic or chemical features in grow-then-place approaches. For many applications it is important that these placement cues themselves have nano-scale dimensions and spacings. Integration of nanomaterials into complex systems therefore requires nano-scale patterning techniques.

Self-assembly processes are processes that lead to natural two- or three-dimensional organization of structures. Examples include phase separation by nucleation and growth or decomposition of unstable structures, as well as monolayer formation and dewetting. These self-assembly processes often lead to structures that are locally ordered at length scales which can not be readily obtained through lithographic techniques. However, self-assembly processes do not lead to structures with long-range order and generally do not

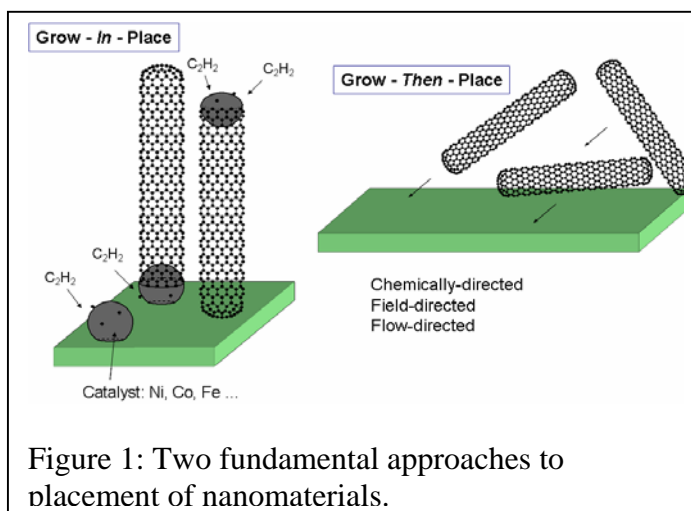


Figure 1: Two fundamental approaches to placement of nanomaterials.

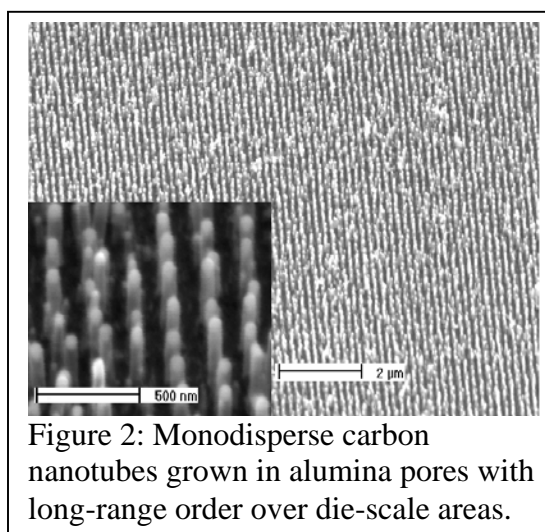


Figure 2: Monodisperse carbon nanotubes grown in alumina pores with long-range order over die-scale areas.

lead to ordering in controlled or predictable locations. An important approach to controlling self-assembly processes is to use lithographically defined features to provide a template. This allows deterministic location of the ordered features, and can also be used to force long-range order and control the ordering characteristics such as symmetry and period. The combination of lithography and self-assembly allows ordering of materials with sub-lithographic dimensions, and at sub-lithographic spacings.

Several groups at MIT have collaborated with MIT's Nano-structures Laboratory to demonstrate templated-self assembly (TSA), and to use TSA as a route to creation of systems of organized nano-materials. Several examples from this work will be briefly discussed. These will include:

- i) Templating of block co-polymer phase separation to ultimately produce ordered arrays of nano-magnets, with sub-lithographic dimensions and spacings [2];
- ii) Templating of pore formation in anodized alumina to produce ordered pores with sub-lithographic dimensions that are used as scaffolds for nano-wire and nano-tube growth (Figure 2)[3]; and
- iii) Templated solid state dewetting to produce catalyst arrays [4].

These examples will be used to illustrate general principles that can be applied to other processes and applications.

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THE EUROPEAN UNION'S 7TH FRAMEWORK PROGRAMME: NMP PRIORITY

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The Commission's proposal for the Seventh Framework Programme (FP7)², published 6 April 2005, provides a coherent and ambitious pan-European framework for supporting Research, Technology and Development (RTD) as part of the research policy and constitutes a 7-year strategic plan for the period 2007-2013. In addition to its relevance to the building of a European Research Area (ERA)³, FP7 is one of the initiatives linked to the Lisbon agenda for European growth and competitiveness⁴; along with a new Competitiveness and Innovation (CIP), Education and Training programmes, and Structural and Cohesion Funds for regional convergence and competitiveness.

In the Commission's Communication 'Building the ERA of knowledge for growth'⁵, which accompanies the FP7 proposal, the central importance of research is stressed. Research is a key component of the 'knowledge triangle' along with education and innovation, and is at the core of the EU's strategy to create growth, competitiveness and employment while maintaining social and environmental sustainability. To be a genuinely competitive, knowledge-based economy, Europe must become better at producing knowledge through research, at diffusing it through education and applying it through innovation.

The proposed FP7 addresses the six main objectives of the new EU research policy⁶ in four specific programmes: Cooperation, Ideas, People and Capacities. In the Cooperation programme, with more than half the total FP7 budget, support will be provided to transnational cooperation at every scale across the European Union and beyond, in a number of thematic areas corresponding to major fields of the progress of knowledge and technology, where research must be supported and strengthened. Across all these themes, support to transnational cooperation could be implemented through: Collaborative research, Joint Technology Initiatives and/or Technology Platforms, Coordination of non-Community research programmes (including ERA-NET) and International Cooperation.

The Ideas programme will set up a European Research Council to stimulate creativity and excellence of European research by funding basic or 'frontier' research by individual teams competing at European level. The People programme will develop and strength, quantitatively and qualitatively, the human potential in research and Technology in Europe by putting into place a reinforced and coherent set of 'Marie Curie actions'. And, finally, the Capacities

¹ The present paper does not represent any commitment on behalf of the European Commission

² <http://cordis.europa.eu.int/fp7/>

³ <http://www.cordis.lu/era/>

⁴ <http://europa.eu.int/growthandjobs/>

⁵ <http://icadc.cordis.lu/fep->

[cgi/srchidadb?ACTION=D&SESSION=&DOC=1&TBL=EN_DOCS&RCN=6798&CALLER=FP7_LIB](http://icadc.cordis.lu/fep-cgi/srchidadb?ACTION=D&SESSION=&DOC=1&TBL=EN_DOCS&RCN=6798&CALLER=FP7_LIB)

⁶ ftp://ftp.cordis.lu/pub/era/docs/com2004_353_en.pdf

programme will enhance the research and innovation capacities throughout Europe by coordinating and developing research infrastructures of European interest and by supporting regional research-driven clusters, SMEs, a closer relationship between science and society, and the development of international cooperation.

While building on the achievements of its predecessor, FP7 shows substantial continuity but includes new elements: emphasis on research themes; significant simplification of its operation; focus on developing research that meets the needs of European industry, through the work of Technology Platforms and the new Joint Technology Initiatives; establishment of a European Research Council, funding the best of European science; integration of International cooperation in all four programmes; development of Regions of Knowledge, a Risk-Sharing Finance Facility aimed at fostering private investment in research.

The nine themes covered in the Cooperation programme present strong elements of continuity with its predecessors in FP6 and correspond to major fields in the progress of knowledge and technology, where research must be supported and strengthened to address European social, economic, environmental and industrial challenges. These themes are broadly defined in both the FP7 proposal and the Commission's proposal for the Specific Programmes²

Theme 4, 'Nanosciences, Nanotechnologies, Materials and New Production Technologies' (NMP), has as overall objective to improve the competitiveness of the European industry (including SMEs) and ensure its transformation from a resource-intensive to a knowledge-intensive industry, by generating breakthrough, applicable, knowledge for new applications at the crossroads between different technologies and disciplines. A key element of this theme is the effective integration of nanotechnologies, materials sciences and new production methods so as to achieve and maximise the impacts for industrial transformation and, at the same time, supporting sustainable production and consumption. The theme will support all industrial activities operating in synergy with other themes. Strong contribution to industrial needs and complementarities through initiatives and funded projects will be ensured in particular through European Technology Platforms by means of their Strategic Research Agenda that would help to establish common research priorities.

Nanosciences and Nanotechnologies (N&N) will have an important role in FP7. Advances across a wide range of sectors are being enabled through R&D in N&N. These advances can address the needs of citizens and contribute to the Union's competitiveness and sustainable development objectives and many of its policies including public health, employment and occupational safety and health, information society, energy, transport, security and space. FP7 will be the main initiative for implementing the Action Plan on Nanosciences and Nanotechnologies⁷ that was approved by the Commission in June 2005. The NMP priority will host most of the research on N&N that, however, may well be carried out also within IST funding chapters for applications in electronics and photonics.

More detailed research domains will be defined through open calls for proposal. The first call in FP7 is expected to be launched at the end of 2006; however both the FP7 and the Specific Programmes have still to be approved (by a co-decision procedure for FP7 and by the Council following opinion by the European Parliament for the Specific Programmes).

⁷ <http://cordis.europa.eu.int/nanotechnology/actionplan.htm>

ATOMIC PROCESSES ON CATALYST SURFACES: MANY-BODY INTERACTIONS AND HIGH PRESSURE EFFECTS

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We are using STM to investigate catalytic reactions on metal surfaces. By resolution of adsorbed atoms and molecules we can get new insight into elementary catalytic processes, such as the dissociation of molecules at "active sites" and reactions between adsorbed particles. In this way catalytic reaction models can be tested by direct imaging. In all cases studied so far we have observed much more complex surface processes than previously assumed.

In this talk I will focus on two examples from our recent work. We have investigated interactions between adsorbed atoms in great detail, because it was found that spatial distributions strongly deviate from statistical distributions, which, in turn, have strong effects on reactions rates. We find that interactions between particles are not strictly pair-wise, but that significant many-body interactions have to be included. The resulting configurations have been imaged for the first time in thermodynamic equilibrium. The findings are in good agreement with DFT calculations and Monte-Carlo simulations.

In the second part I present first results obtained with a newly developed STM for high pressure investigations. The setup allows us to perform experiments under pressure and temperature conditions that come close to those of industrial catalytic processes. Atomic resolution is still achieved. We hope in this way to bridge the so-called pressure gap between surface science and applied catalysis, one of the fundamental problems in catalysis research.

Pamplona 20-23, March 2006



3rd NANOSPAIN WORKSHOP

ORAL CONTRIBUTIONS

SYNTHESIS OF SILVER NANOPARTICLES WITH GREAT MONODISPERSITY AND LONG-TERM STABILITY IN AQUEOUS SOLUTION

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Nanoparticles of noble metals have received great interest due to properties associated to their nanometer dimensions. These differ widely from those of the bulk metal as a consequence of electron confinement and quantum size effects.

Gold nanoparticles have been extensively investigated [1] due to their chemical inertness but silver nanoparticles show better optical properties due to the sharpness of their plasmon absorption band at wavelengths that are strongly dependent on the medium in which the particles are present.[2] This sharp plasmon resonance has been employed for the enhancement of Raman signals (SERS) [3] or for replacing fluorescence markers of biological events.[4] These applications require aqueous Ag colloidal solutions. However, silver is chemically more reactive than gold and therefore, a general aim of synthetic efforts is to produce these nanoparticles with a narrow and controlled size distribution and employing capping ligands that can provide long-term stability toward oxidation.

Most of the preparative methods that have been previously reported employ the reduction of Ag⁺ salts by sodium borohydride [5] or sodium citrate [6] in an aqueous phase and their stabilization by protecting agents such as citrate [7], surfactants [8] or thiols [9]. These methods generally produce mainly small particles but most of them lack size monodispersity or stability. By contrast, preparation carried out in an organic phase [10] based on reverse micelles yield better particle monodispersity and higher particle concentrations than water-based preparations. The two-phase synthetic route for preparing monolayer protected clusters (MPCs) of gold has also been used for silver. [11] Once synthesized, efficient transfer of the colloid to an aqueous medium by the use of capping ligands providing stability to the nanoparticles is required. Different strategies based on thiol chemistry has been attended for this purpose.[12] In this way, thioctic acid (TA) has been successfully employed recently as a ligand for gold MPCs and appeared therefore, to provide excellent stability for the stabilisation of silver particles. [13]

This communication reports the synthesis of monodisperse silver nanoparticles in an organic phase and their subsequent efficient transfer to water using TA to obtain stable colloidal preparations (Fig. 1).

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Figures:

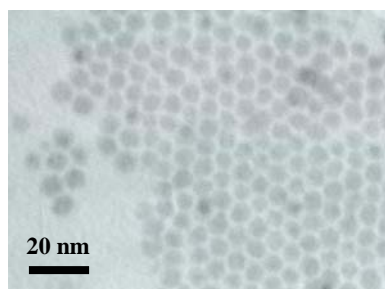


Fig.1. TEM picture of Thioctic acid-derivatized silver nanoparticles.

MECHANICAL PROPERTIES OF SUSPENDED ATOMIC CHAINS OF GOLD

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The mechanical properties of matter in the nanometer scale and their relation to electrical properties are of great interest both from a fundamental point of view and for future nanotechnological applications. Particularly simple and appealing model systems are the freely suspended single-atom chains of various metals that form spontaneously as a contact of nanometer dimensions is pulled apart [1,2]. Gold atomic chains are very stable at low temperatures and offer the possibility of studying the mechanical behavior of a small number of atoms in a well-defined configuration. In a previous work [3] we directly measured the forces during the pulling of these chains and, in particular, the breaking force, using a deflection sensor. A drawback of this method is that a large part of the deformation during the pulling is taken up by the electrodes precluding a measurement of the elasticity of the chain as a function of elongation. In contrast, the electron-phonon interaction can be used to probe the elastic properties of the atomic chains [4] independently.

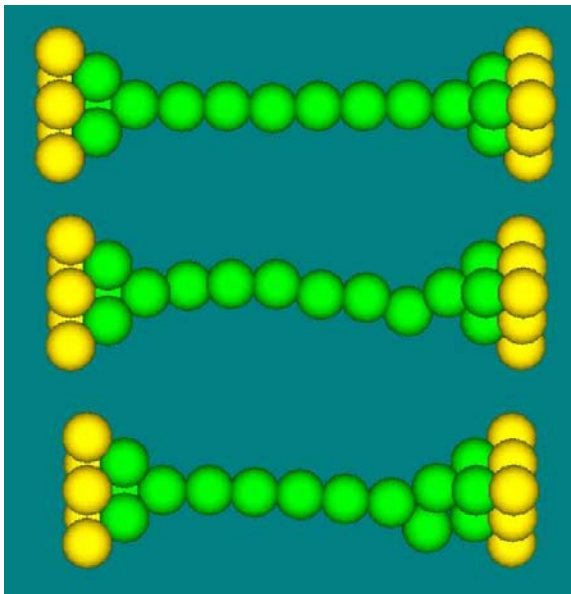


Fig. 1. Molecular dynamics evolution of a suspended atomic chain of gold atoms during compression. The interaction between the Au atoms is modelled using a Finnis-Sinclair potential. The chain is observed to decrease in length atom by atom.

In this work, we study experimentally the response to strain of suspended atomic chains of gold by following the differential conductance and using the electron-phonon interaction as a probe. In contrast to previous experiments [3,4] the atomic chains are compressed instead of elongated, which makes possible to follow the process from a well defined starting situation. In order to gain some insight into the relevant atomistic mechanisms, we also perform extended molecular dynamics simulations, using a Finnis-sinclair potential, of this process.

We find that during compression the atomic chains contract atom by atom and discuss the mechanism for this particular process. We are also able to extract the dependence on the interatomic distance of the elastic constant of the chains.

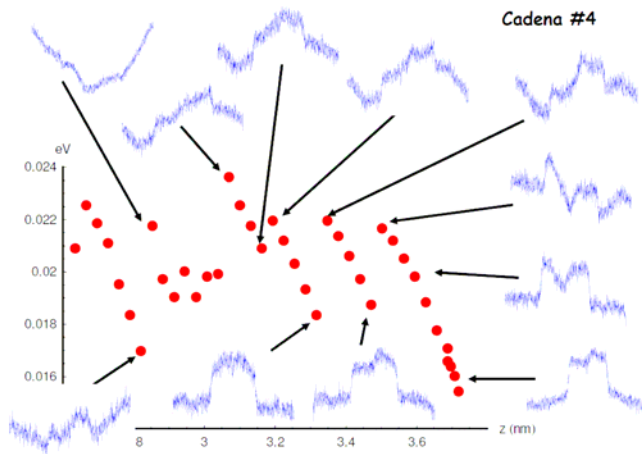


Fig. 2. Experimental evolution of the differential conductance of an atomic chain during the compression process. The sharp drops in differential conductance due to electron-phonon scattering are clearly visible.

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HIGH RESOLUTION OPTICAL SPECTROSCOPY OF SINGLE SELF-ASSEMBLED QUANTUM DOTS AND RINGS

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The electronic and optical properties of self-assembled quantum dots (QDs) have been intensively studied over the last years attending to both, their collective behavior in ensemble averaged experiments, and their individual properties using single QD spectroscopies. The studies reveal that an atomic-like density of states is well suited to describe the ground and first excited states of these nanostructures. In such situation, the creation and annihilation of multiparticle exciton complexes are dominated by the *Coulomb blockade* and the *Pauli exclusion principle*, being the direct and exchange coulomb interaction energies much larger than typical homogeneous linewidths in the system. A discrete electronic structure is necessary to allow for coherent control of individual spin and/or charge states and fulfil the requirements of quantum information applications. Indeed, simultaneous optical and electrical access to single QDs have been demonstrated and successfully applied to implement solid state based quantum gates, or to fabricate novel devices like single photon emitters.

In spite of this success, the artificial atom picture overlooks many properties inherited by the QD from its embedding semiconductor matrix. The interaction between the discrete QD band structure and the different matrix-related-continua is responsible for a number of electronic and optical properties that are not simple extrapolation of a discrete density of states.

In order to establish a complete and unified picture, systematic studies based in nanostructures with different size, shape and composition are desirable. But, to accomplish this, high resolution spectroscopic techniques are necessary to give the necessary insight in the spatial, spectral and temporal domains.

In this talk we will present our most recent developments in the confocal spectroscopy of single quantum dots and rings addressing many of the issues above mentioned. The stress will be given to show how is possible to determine the electronic structure of individual quantum nanostructures by using novel emission, excitation, absorption and reflection spectroscopy techniques.

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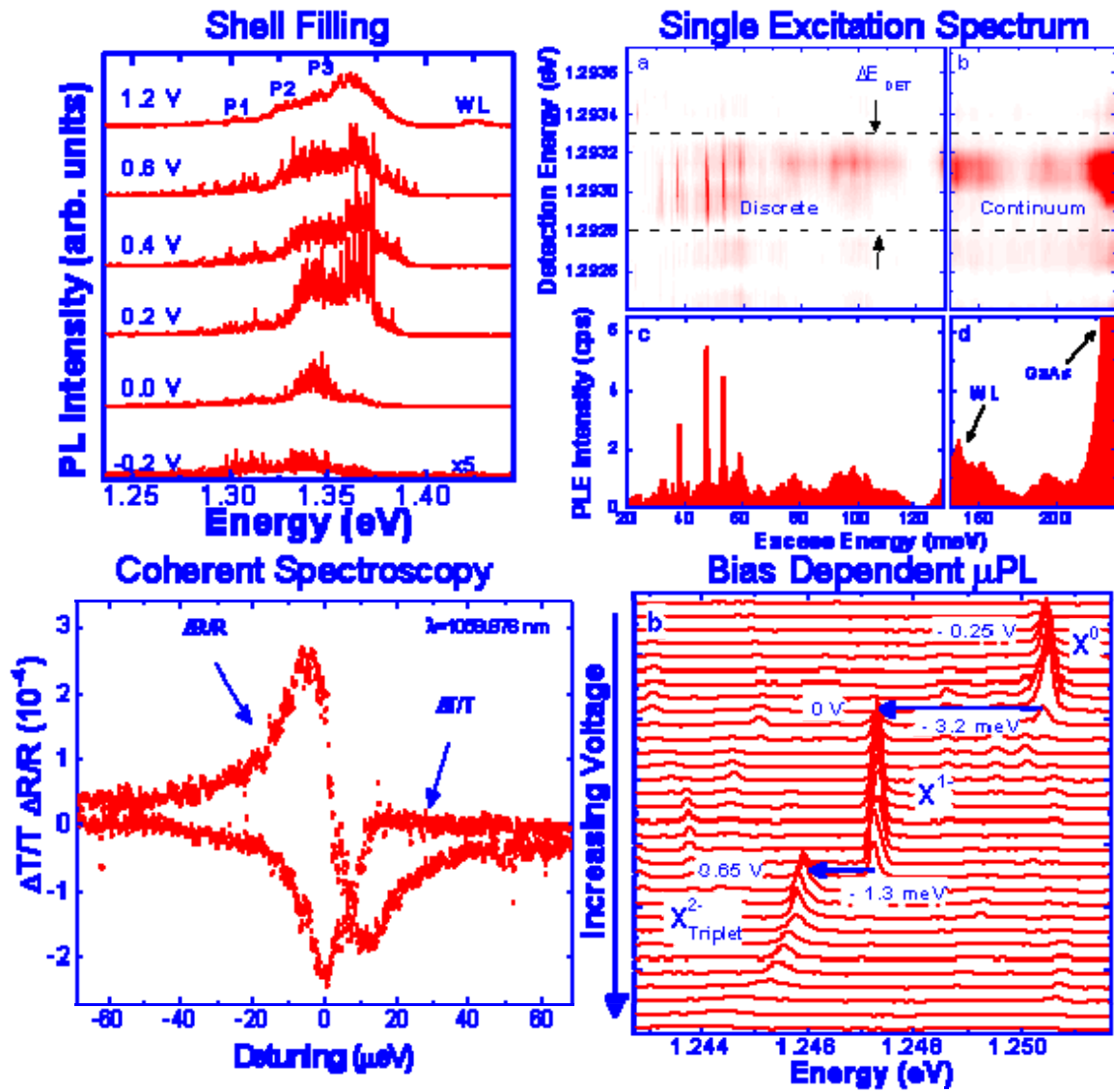
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Figures:

The result of four different experiments will be shown to reveal the complex nature of the electronic structure of self-assembled single quantum dots and rings.



NANORESONATORS WITH INTEGRATED CIRCUITRY FOR HIGH SENSITIVITY AND HIGH SPATIAL RESOLUTION MASS DETECTION

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In this contribution we will summarize the main results achieved during the development of the Nanomass II project funded by the European Community under the “Information Society Technologies” (IST-2001-33068). The objective of Nanomass II project is the development of the technologies for the combination of CMOS circuit fabrication with nanotechnology processes and techniques. The technology will be applied to the realization of mechanical mass sensors based on resonant nanometer scale silicon cantilevers integrated monolithically with the CMOS signal conditioning circuits. The excitation and detection of the cantilever displacement will be performed through the monolithically integrated CMOS circuitry.

Mass detection is based on monitoring the resonant frequency shift of the cantilever when nanometer-sized particles or molecules are deposited on the cantilever. The cantilever is electrostatically excited by means of an electrode located at submicrometer distance from the cantilever. A change in the cantilever resonance frequency is detected as a capacitance change. Electrostatic transduction in the nanometer-size regime requires the minimization of the parasitic capacitance since the magnitude of the current to be detected is proportional to the coupling capacitance between the cantilever and the driver, which is in the order of 10^{-17} F. Consequently, the readout circuitry has to be integrated “on-chip” in order to eliminate the parasitic capacitance introduced by the external bonding pads and wires. CMOS circuitry for excitation and read-out of the cantilever deflection is integrated together with the cantilever by using a monolithic technology that consists of the combination of standard CMOS processes and novel nanofabrication methods.

As a result of the developments pursued in the project a full System-on-Chip based on a nanoelectromechanical device and its read-out circuitry has been obtained. Figure 1.1 schematizes the main result achieved as a System-on-Chip. From the sensor point of view, a new type of high performance sensor devices capable of measuring one single molecule (i.e. a medium size protein as polypeptide chains) is expected: the resulting devices can be used as mass sensors, with an expected mass resolution of 10^{-19} g in vacuum, and a spatial sensitivity of less than 100 nm.

In particular, the project has developed the technology to combine standard CMOS technology with nanofabrication of resonant cantilevers. This includes nanocantilever fabrication using different techniques for nanofabrication: (i) laser/AFM nanolithography; (ii) electron beam nanolithography (EBL) and (iii) nanoimprint lithography (NIL), and its combination with CMOS integrated circuitry for the electrical readout and signal conditioning. The different nanolithography processes have been compared in order to evaluate the advantages of these techniques in terms of dimensions reduction, throughput and CMOS compatibility.

From the point of view of the material to fabricate the resonant cantilever, three approaches have been established: a) use of a polysilicon layer from the CMOS technology, b) use of crystalline silicon from SOI wafers and c) metal deposited by electroplating. The compatibilization with CMOS has provided the best results on polysilicon. On the other hand, the improvement on the mechanical properties of the cantilever resonator using crystalline silicon and the possibility to achieve smaller widths than with polysilicon (due to its granular structure), give to the SOI approach an added value to be taken into account. Concerning the metal cantilevers, preliminary results made on non-integrated devices have shown a good resonant behavior and mass sensitivity. Integration into CMOS has not been attempted because of time constraints.

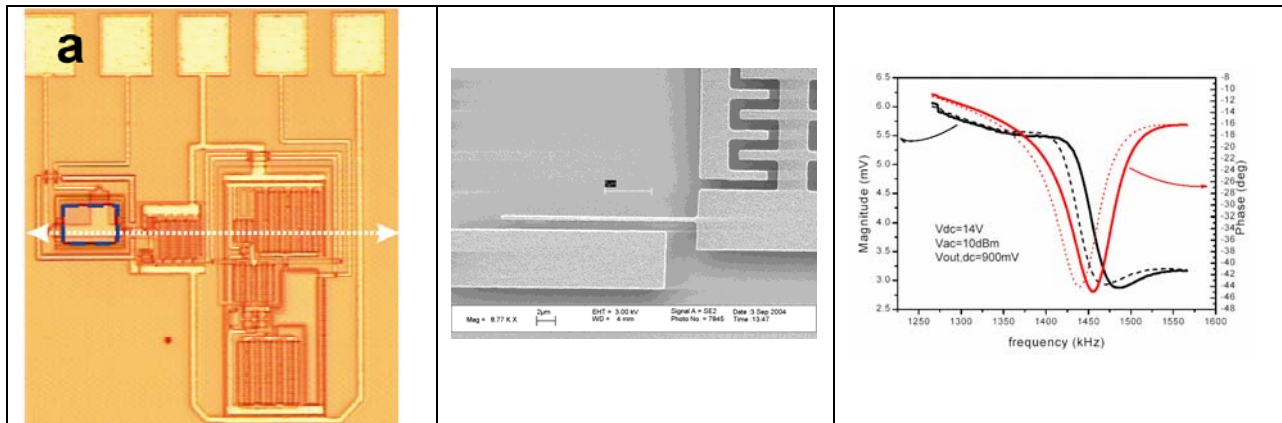


Figure 1.1. System-on-chip fabricated sensor: a) optical image of the CMOS read-out circuit and the area in which the nanoresonator will be fabricated (blue square); b) scanning electron microscopy of a nanocantilever fabricated using electron beam lithography on the CMOS substrate; c) read-out obtained from the CMOS circuitry of the oscillation of the cantilever before mass deposition (solid line) and after mass deposition (dotted line).

During the course of the project several demonstrators have been fabricated, which show the relative performance of each technological approach (from the point of view of the fabrication technique and also from the point of view of structural material for the cantilever):

i) Sensor formed by a single nanometer scale cantilever using Polysilicon as structural layer and laser lithography for defining the cantilever integrated monolithically with the CMOS read-out circuit. The dimensions of the cantilever are: length, $l=40\ \mu\text{m}$; width, $w=840\ \text{nm}$; thickness, $t=600\ \text{nm}$ and gap spacing $s=1.3\ \mu\text{m}$. The natural resonance frequency derived from the experimental measurements is 703 kHz. The theoretical sensitivity of this cantilever is $34 \cdot 10^{-18}\ \text{g/Hz}$, which is an extremely high sensitivity for punctual mass detection. In terms of distributed mass detection, the sensitivity is $12 \cdot 10^{-13}\ \text{g/Hz/cm}^2$ which is comparable to quartz microbalances. In this first demonstrator the minimum measurable frequency change due to the electrical noise of the CMOS integrated circuitry and assuming that any measurement will be made in air (low Q factor) is $\delta f \approx 1.9\ \text{Hz}$. In this case, the final mass sensitivity with the integrated system is below 65 attograms.

ii) Sensors formed by a single nanometer scale cantilever using Polysilicon as structural layer and fabricated by electron beam lithography integrated monolithically with the CMOS read-out circuit. The cantilever width is 420 nm, the thickness is approximately 600 nm and the length is 20 μm . The natural resonance frequency derived from the experimental measurements is 1.42 MHz. From the experimental mass measurements performed with this integrated NEMS sensor a mass sensitivity of approximately 3 ag/Hz has been determined.

iii) Sensors formed by a one-dimensional array of polysilicon cantilevers fabricated by standard optical lithography integrated monolithically with the CMOS read-out circuit. In this demonstrator, arrays of 2, 4 and 8 cantilevers with different excitation and detection schemes have been obtained. The dimensions of the cantilevers are 50 microns long, 1.4 microns wide and 600 nm thick. The natural resonance frequency of these cantilevers is around 750 kHz and its mass resolution is 63 ag/Hz. In this case the demonstrator will be useful for applications in which high mass sensitivity and multiple detection is needed (i.e. specific detection of different molecules simultaneously), or when a spatial extended map is required (for example, mapping of an atom beam). It will allow performing additional signal processing like for example differential reading. It will also be possible to implement redundancy (multiple detection of the same magnitude) and interchangeability, which will increase the robustness and yield of the device.

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WATER SOLUBLE MAGNETIC GLYCONANOPARTICLES: SYNTHESIS, CHARACTERIZATION, CELL RESPONSE AND APPLICATIONS AS CONTRAST AGENTS FOR MRI.

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Nanometer-sized particles have been focus of intensive research over the last 20 years [1]. This interest is stimulated from their technological importance, as they exhibit unique electrical, optical, and magnetic properties, which differ from their respective bulk. Such novel properties provide the potential for huge improvements in biomedical sciences including detection, diagnosis, and therapeutic systems [2]. Magnetic nanoparticles offer exciting new opportunities including improving the quality of magnetic resonance imaging (MRI), hyperthermic treatment for malignant cells, site-specific drug delivery and also the recent research interest of manipulating cell membranes [3]. Previously reported magnetic nanoparticles with tailored surface chemistry have been widely used experimentally for numerous *in vivo* applications. The biological applications of these nanomaterials require that these nanoparticles must have high magnetization values, size smaller than 20 nm, narrow particle size distribution and a special surface coating to avoid toxicity and biocompatibility problems, but also to target the desired area. The development of functional magnetic nanoparticles is mainly based on proteins and nucleic acids. However, as far as we know, magnetic nanoparticles conjugated to biologically relevant oligosaccharides for specific cell targeting have not yet been prepared.

Our laboratory has recently been successful in preparing gold nanoclusters and semiconductor nanocrystals functionalized with carbohydrate antigens (*glyconanoparticles*) [4]. These carbohydrate functionalize gold nanoclusters have been shown to be excellent platforms for basic studies of carbohydrate interactions and potential tools for biotechnological and biomedical applications [5]. We also explored the potential of these tools for cell labeling and imaging of carbohydrate-mediated biological processes. To this end, we propose the use of magnetic glyconanoparticles as potential targetable MRI agents.

Therefore, in this study, magnetic gold-iron nanoparticles coated with different saccharides (glucose, maltose and lactose) have been prepared using a straightforward and economical methodology. They have been characterized by ¹H-NMR, UV-vis, AFM and TEM.

Magnetization curves as a function of the applied field at different temperatures, as well as the dependence of magnetization with the temperature have been measured for the Au-Fe MG NPs as well as for the iron free Au GNPs. It was very exciting to observe a ferromagnetic behavior not only for the AuFe MG NPs but also for the iron free Au GNPs [6].

The influence of these nanoparticles on human dermal fibroblasts *in vitro* has been assessed in terms of cytotoxicity, light microscopy and scanning electron microscopy (SEM). From the results, we observed that, although **maltose-MGNP** presents an extremely high cytotoxicity, lactose and glucose are innocuous. We have also observed that lactose and **maltose-MGNPs**

are able to internalize the cell membrane via endocytosis, but this effect was not detected for **gluco-MGNPs**.

This kind of polyvalent magnetic glyconanoparticles complements the presently available bioactive iron oxide nanoparticles. Their easy preparation and purification, their small core size, their stability and solubility in physiological conditions as well as their biocompatibility, convert these tools in potential candidates for MRI applications.

To confirm this application, the longitudinal (spin-lattice) and transversal (spin-spin) relaxation times (T1 y T2) of our MGNPs were measured. All the MGNPs showed similar relaxivities and they have an acceptable value, despite to the low content in iron in all of them. Preliminary *in vivo* experiments have also been carried out with **gluco-MGNPs** to demonstrate their utility as agent contrast for tumoral processes. The MGNPs could cross the Blood Brain Barrier and their accumulation in brain tumours allowed their visualization by MRI.

All these experiments have demonstrated the potential application of these magnetic glyconanoparticles in Biomedicine.

Acknowledgments: This work was supported by MEC. JMF and DA thank the MEC for a Ramon y Cajal grant and a predoctoral fellowship respectively. We thank Dr. T.C. Rojas and Prof. A. Fernández for their help with the TEM images.

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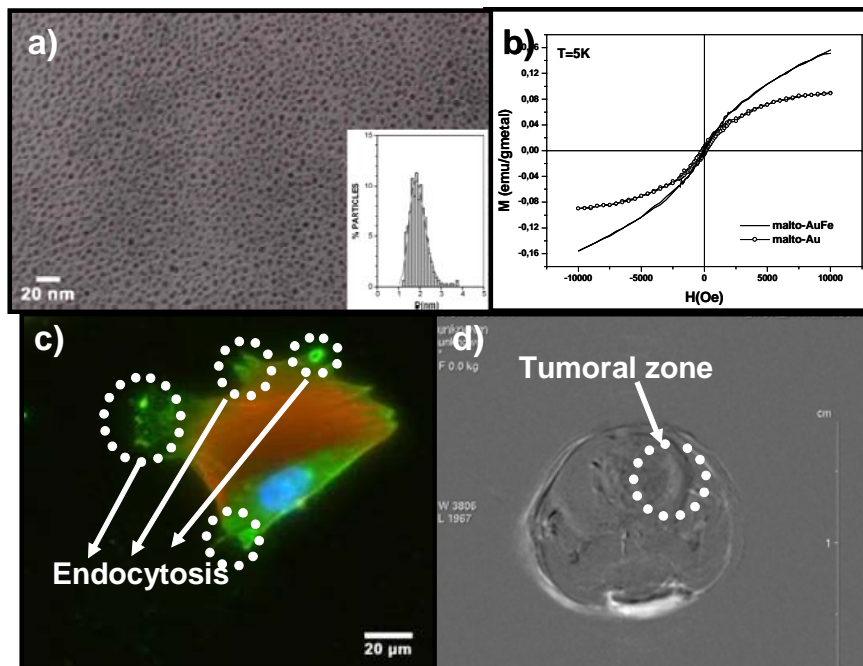


Figure 1: a) TEM micrograph and core size-distribution histograms of **lacto-MGNP**, b) Magnetization curves at 5 K for **malto-MGNP** and **malto-Au**, c) F-actin and clathrin fluorescent staining for cells incubated with **lacto-MGNP**, d) *in vivo* experiments of **gluco-MGNP** as contrast agents.

Understanding carbon nanotube growth with photoelectron spectroscopy

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The degree of growth control necessary to fulfill the huge potential of carbon nanotubes (CNTs) for a big number of applications requires a deep knowledge of the factors involved in the growth process. We have undertaken to study the role that the catalyst chemical state plays in the growth of CNTs, using chemical vapor deposition (CVD) and supported catalyst growth methods. We have been in an almost unique position to do so, combining previous experience in the deposition of diverse nano-structured thin films with *in situ* chemical characterization by photoelectron spectroscopy. We have developed an experimental setup, which allows for the characterization of CNT samples at any stage of the growth, without need to expose the samples to air at any moment. Control on the chemical composition of substrates and catalysts is guaranteed by sequential deposition of materials and final CNT growth in the same closed vacuum environment. Although we have by no means answered all questions related to the complex factors involved in the CNT growth, we have obtained important information concerning the role of the support in the morphological and chemical evolution of a Fe catalyst during the process, and its ultimate influence in CNT growth rates and morphological characteristics. In particular, we could establish that *the oxidation state of the Fe catalyst is one of the key factors controlling the structure and growth mode of CNTs*. [1]

We have determined that the use of Al₂O₃ buffer layers is linked to a transformation of the original metallic iron film to Fe₂O₃ particles. These particles remained oxidized in the form of FeO even after interaction with the reducing atmosphere of hydrogen-rich byproducts of the decomposition of acetylene after the start of the CVD process. In the growth catalyzed by FeO onto Al₂O₃, we have observed the formation of thin tubes with a low number of poorly graphitized walls (2-5), a comparatively fast growth rate and high density of nanotubes. With these experiments we have shown that iron oxide particles can efficiently catalyze CNT growth. This is an important observation, because it implies that in this case CNT growth has not proceeded through a bulk diffusion step of the carbon atoms since dissolved C would result in the immediate reduction of FeO to metallic Fe.

In the case of the TiN and TiO₂ films, although there is initially a partial oxidation of the iron catalyst after the annealing procedure, iron was observed to revert to its original metallic state after interaction with acetylene. When the growth is associated with formation of metallic Fe particles onto TiN or TiO₂, it proceeds at a slower rate, and the CNTs formed are thick multi-walled nanotubes (20-40 walls), with a better graphitization of the walls but more twisted structures (bends, bamboo-like inner structures, etc). All these differences accumulate to suggest different growth mechanisms involved in the two cases.

Additionally, we have proven that Ultra-Violet photoelectron spectroscopy (UPS) can successfully be applied to CNTs in order to extract information about diameter distribution [2]. Since this technique also provides first hand information on the effect that experimental parameters have on the diameter distribution of different samples, it is an interesting

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alternative/complement to other ex situ characterization techniques, like for example Raman spectroscopy (in particular in order to speed up the process of finding the appropriate experimental conditions).

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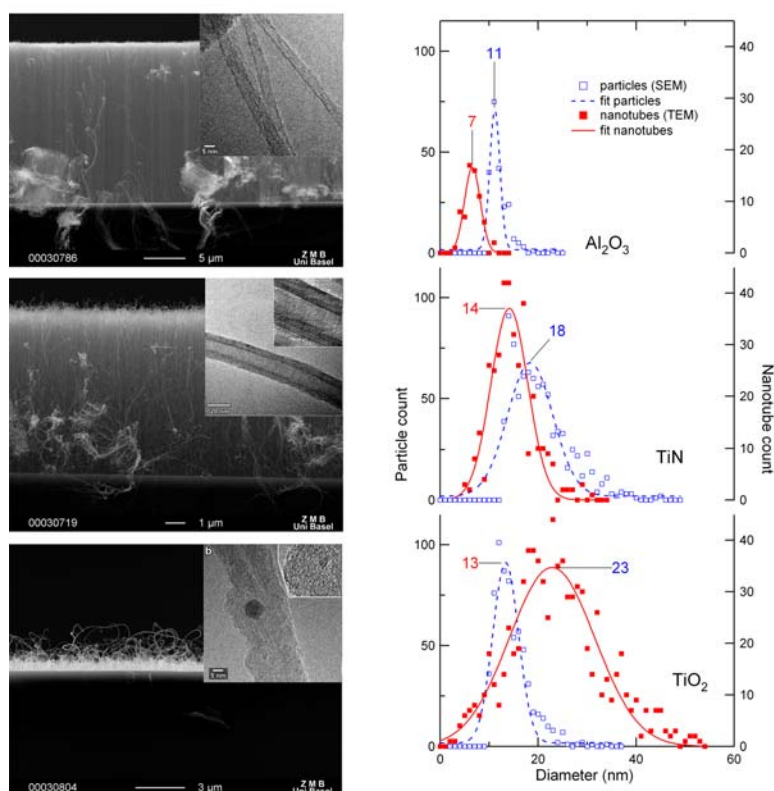


Figure: Left: TEM and SEM images of carbon nanotubes grown under identical experimental conditions onto Si wafers covered with buffer layers of Al₂O₃, TiN and TiO₂ (from up to down). Right: diameter distributions of initial catalyst particles and the final CNTs. The broader CNT diameter distribution in the case of TiO₂ grown tubes could be an indication of further particle evolution and coalescence even after the CVD start.

ULTRAFAST DYNAMICS OF CdTe NANOPARTICLES IN WATER SOLUTION

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Within recent years, we have reported on fast and ultra fast events in chemical and biological nanocavities.[1-5] As expected,[6] the results obtained demonstrated that confinement may affect both spectral (color) and time domains. Here we continue our efforts in studying ultrafast dynamics in confined systems by reporting on the first femtosecond observation of CdTe nanoparticles relaxation in water solutions. We used two different CdTe nanoparticle colloids with size of 3 and 5 nm, and the fs-up conversion technique to interrogate their behaviour at different emission observations. We studied also the excess energy of excitation and the effect of deuterium on the observed relaxation times. We found a rich dynamics with times ranging from 50 fs to 10's of ps, and explain the results in terms of hole-electron combination and ultrafast relaxation to the ground states. As these nanoparticles are currently used for cancer photodetection, we believe that these results might be important for a better understanding of nanoparticles behaviour in biological media and for the development of nanobiotechnology.

Acknowledgements: This work was supported by the MEC and JCCM through the projects: MAT2002-01829, SAN-04-000-00 and PBI-05-046.

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PREPARATION OF MESOPOROUS SILICA WITH SMALL PORE SIZE AND THICK WALLS, BY USING FLUORINATED SURFACTANTS

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Many mesoporous materials, such as the MCM-41 type prepared by using cationic surfactants, are not hydrothermally stable because of thin pore walls [1-3]. A great interest has been focused on the preparation of robust materials with controlled pore size and morphology [2-8]. In this context, materials with large pores and thick walls, such as the SBA-15 type, have been prepared using nonionic copolymer surfactants [6-8]. However, robust materials with small pore sizes, of great scientific and technological interest, have not been described yet. In the present work, mesoporous silica with small and thick pore walls has been obtained using fluorinated surfactants as templating systems [9]. This type of surfactant, due to their strong lipophilic character, forms smaller aggregates than those with conventional hydrocarbon chains. The mesoporous silica was prepared by precipitation in fluorinated surfactant aqueous solutions, and the resulting materials were characterized by small angle X-ray scattering, transmission electron microscopy and nitrogen sorption isotherms. The results showed that the concentration of surfactant required to obtain well-ordered mesoporous materials was very low (1 wt%), and the pore walls were thick ($> 20 \text{ \AA}$). Two-dimensional hexagonal (p6mm) mesostructure was obtained at HCl concentrations higher than 0.1 M, whereas disordered worm-like mesostructured silica was formed at lower HCl concentrations. The nitrogen sorption determinations showed high specific surface areas (around $1000 \text{ m}^2 \text{ g}^{-1}$) and very homogeneous inner pore diameters, in both hexagonal and worm-like materials. The mesostructure was robust and the specific surface area was not affected by calcination at high temperature, despite a small reduction (approximately 2 \AA) in d-spacing. All these results demonstrated that fluorinated surfactants are very appropriate for the preparation of mesostructured materials with small pore diameters and thick pore walls.

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SYNTHESIS OF MAGNETIC NANOSTRUCTURED SILICA-BASED MATERIALS AS POSSIBLE VECTORS FOR DRUG-DELIVERY APPLICATIONS

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In spite of encouraging progress in recent years, the development of magnetic nanoparticles that can be used as drug delivery vectors remains a significant challenge for materials scientists. Among the multiple hurdles that must be overcome are the provision of a sufficiently high magnetic response, a high loading capacity for therapeutic or diagnosis materials and a sufficient degree of biocompatibility. Here we describe the preparation of encapsulated magnetic nanoparticles within silica shells using three synthesis methods: *i*) the arc-discharge method, *ii*) mechanical activation using high-energy milling at room temperature, and *iii*) by using several cycles of wet impregnation under vacuum of an iron-solution, followed by drying, oxidation and reduction steps.

Conventional cancer treatments include surgery, radiation and chemotherapy. Surgical removal and irradiation are mainly limited by the accessibility to the tumor, while chemotherapy is restricted by the lack of selectivity towards tumor cells, often giving rise to severe side effects in healthy tissues.

Magnetic-controlled drug delivery is a promising alternative to avoid the problems associated to conventional drug delivery methods. In this case, an external or internal magnetic field is used to direct drug delivery vectors to the proximity of the target, therefore enabling significant reductions on the necessary dose of medication and minimizing the unwanted systemic effects [1]. Magnetic drug-delivery vectors consist of a magnetic core and an organic (i.e., polymeric) or inorganic shell with a triple purpose: making the vector biocompatible, avoid clearance by the reticuloendothelial system, and hosting a specific drug by adsorption or encapsulation. The main advantage of inorganic shells compared to organic ones relates to their porous structure, which can often be tailored to control drug loading and drug release rates. In addition, there is no swelling or porosity change with modification of pH, a common problem with organic shells [2]. It is therefore not surprising that the use of particles consisting of a magnetic core and an inorganic shell has been proposed not only for magnetic drug delivery [3] but also for ultra-sensitive disease detection, gene therapy, high-throughput genetic screening, biochemical sensing, and rapid toxicity cleaning [4].

Hence, drug-delivery systems with magnetic nano- and microparticles show a clear potential for cancer treatments in view of advantages such as, *i*) the ability of targeting specific locations in the body, *ii*) the ability of reducing the quantity of drug that needs to be delivered to attain a particular concentration level in the vicinity of the target, and *iii*) the ability of decreasing the concentration of the drug at non-target sites [5].

Here we describe the synthesis of silica-coated iron nanoparticles by means of the arc-discharge method, mechanical activation using high-energy milling at room temperature, and by using several cycles of wet impregnation under vacuum of an iron-solution, followed by drying, oxidation and reduction steps. The first method is a one-step procedure to obtain homogeneous and well-coated particles which, because of their high magnetic response and the rich surface chemistry and physical properties of silica, are promising candidates for their

use in many biomedical applications. In the second method we have used a coating of Y zeolite crystals as an external matrix to prevent magnetite agglomeration as well as to develop a potential host material for magnetic drug-delivery applications. Finally, in the third method, we have developed mesoporous silica particles belonging to the MCM family (MCM-41 and MCM-48), as well as hollow silica microcapsules. Iron was deposited inside the porous structure of both particles and microcapsules in order to obtain magnetic drug-delivery vectors.

Current work at our laboratory is aimed at the functionalization of these particles for drug delivery applications, and more specifically, tumor targeting. The results obtained in this line of research will be presented at the workshop.

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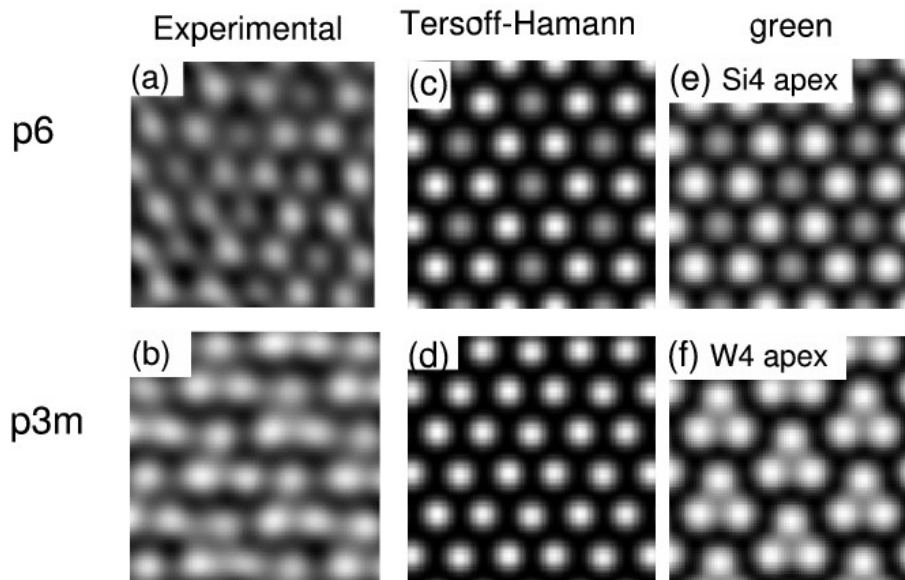
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Subsurface structure of epitaxial silicides imaged by STM

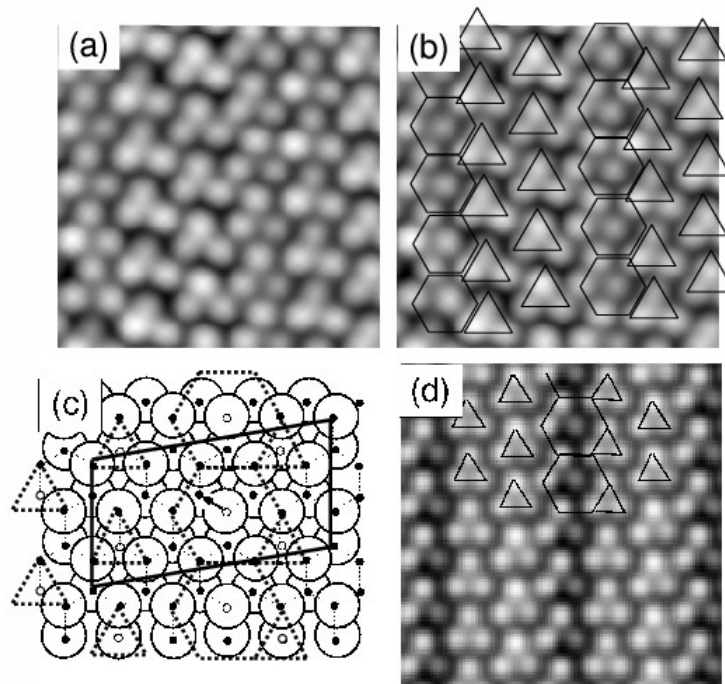
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Via the combination of STM images and *ab initio* calculations we have been able to identify buried vacancies and domain boundaries at the yttrium silicide surface. We find that it is the registry of these vacancies with respect to the almost ideal topmost Si bilayer what determines the symmetry of the STM images, thus allowing to reconcile the two structural models previously proposed for the Rare Earth silicides ($p3m$ and $p6$ models). Our results show that the STM depth sensitivity may reach down to the third layer at a metallic surface, something hardly accessible by other experimental techniques.

Figures:



(2×2) nm² STM images for the surface of the Yttrium silicide: (a) and (b) experimental topographic images exhibiting $p6$ and $p3m$ symmetries, respectively. Tunneling conditions: $I=1$ nAmp, $V=-50$ mV. (c) and (d) Tersoff-Hamann images evaluated 3 Å above the surface for the $p6$ and $p3m$ models, respectively. (e) and (f) theoretical topographic images ($I=1$ nAmp) calculated with a tip (*green* calculation). All theoretical images, (c-f), are calculated for a bias $V=-200$ mV (occupied states).



(a) (10×10) nm² STM image where the $p3m$ and $p6$ patterns are simultaneously imaged. Tunneling parameters: $V = -900$ mV and $I = 0.8$ nAmp. (b) Same as (a) but with the hexagons and triangles drawn on top corresponding to the $p6$ and $p3m$ patterns, respectively. (c) Top view of a defect model. The $c(5 \times 2)$ cell is indicated by the thick solid line, while the expected triangles and hexagons are highlighted by the thick dashed lines. The displaced Si atom at the Y_3Si_5 layer is indicated by a small arrow. (d) Calculated STM topographic image for the geometry depicted in © employing a W4 tip apex ($I = 1$ nAmp, $V = -300$ mV).

NEW METHODS OF FUNCTIONALIZATION OF SINGLE-WALL CARBON NANOTUBES

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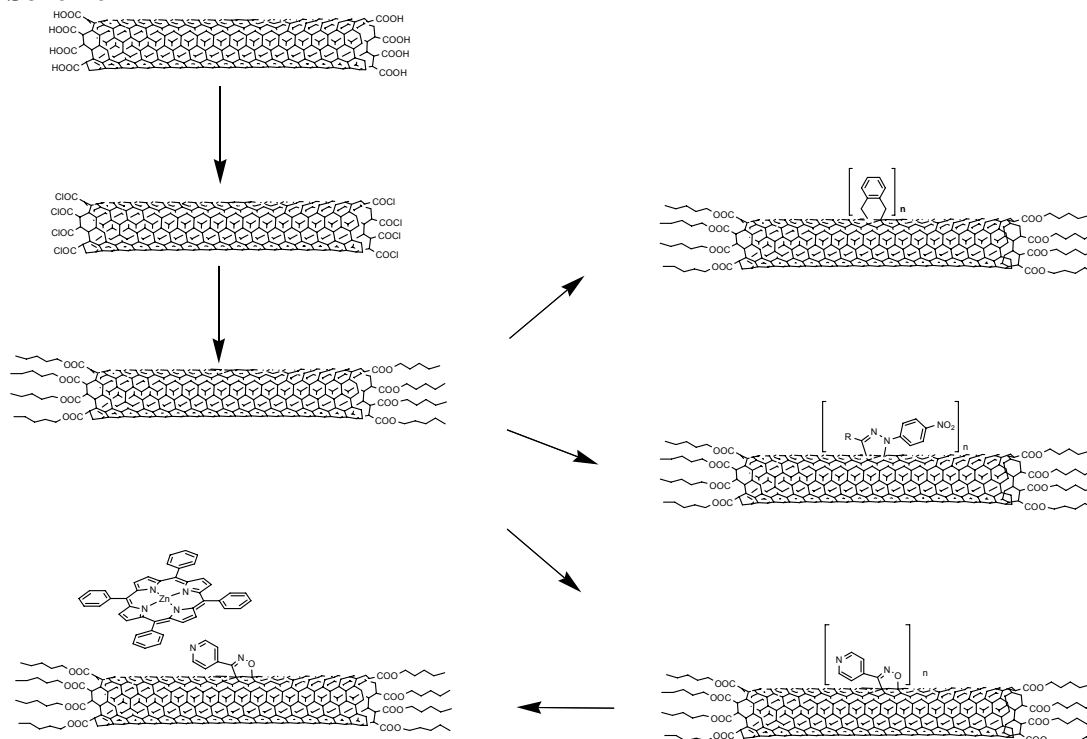
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The past decade has witnessed intensive theoretical and experimental effort toward elucidating the physical properties of single-wall carbon nanotubes (SWNT).[1] Chemical processing and solubility can play an essential role in the applications of this material and over the past few years, interest has focused on their chemical properties and their functionalization is actually a field of great interest.[2] Initially, attempts at functionalization were limited to oxidation reactions [3] to form shortened nanotubes with carboxylic acid groups on open edges. Haddon and co-workers first reported the use of these acid groups to attach long alkyl chains via amide linkages.[4] Later, Sun and co-workers showed that esterification can also be applied to functionalize SWNT.[5]

Covalent chemistry on the walls of the SWNTs is a viable route as well and the achievement of systematic and predictable side wall chemistry is likely to be a precursor to many of the applications envisioned for carbon nanotubes. Recently, reports have appeared on SWNT sidewall functionalizations using fluorine,[6] diazonium salts,[7] nitrenes,[8] and organic radicals.[9] Cycloaddition reactions have proved to be a powerful tool for functionalization of fullerenes and the 1,3-dipolar cycloaddition of azomethine ylides has shown to effective as well in SWNT.[10]

In this communication we show that other cycloaddition reactions employed to functionalize fullerenes as the Diels-Alder reaction of *o*-quinodimethanes,[11] or the 1,3-dipolar cycloaddition on nitrile imines [12] or nitrile oxides [13] can be extended to SWNTs (Scheme.1). The benefits of microwave irradiation as source of energy in these reactions are presented as well. The soluble SWNT derivatives can be characterized by several spectroscopic techniques and show interesting photophysical properties.

Scheme 1



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FIRST-PRINCIPLES SIMULATIONS OF THE CHARGE DENSITY WAVES STM IMAGES OF QUASI-ONE-DIMENSIONAL MATERIALS.

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The Blue Bronze ($\text{Rb}_{0.3}\text{MoO}_3$) and Niobium triselenide (NbSe_3) are layered systems which exhibit quasi-one-dimensional (1D) electron transport properties and metal-semiconductor and metal-metal transitions respectively, to a Charge Density Wave (CDW) phase [1,2].

Despite many attempts, the observation of the CDW phase in Blue Bronze by Scanning Tunneling Microscopy (STM) has been elusive. Only very recently, using a low temperature STM system under ultra-high vacuum, high resolution images have been obtained in which the CDW superlattice was observed, Fig. 1 [3]. However, there are some interesting features of these images which still need to be understood. For instance, what is the effect of the distribution and concentration of surface alkali atoms on the periodicity of the CDW modulation. And why are the most intense features of the observed STM images of the CDW associated with those MoO_6 octahedra that, among the three different types of octahedra in the chain, have the lowest implication in the CDW transition.

In contrast, the CDW phase in NbSe_3 was observed by means of STM long ago [4]. Here, nevertheless, new experimental work [5] has brought some questions which are currently unsolved, such as what is the participation of the type-II chains (from the three in the unit cell) in the CDW modulation.

Here we present first-principles DFT simulations of these systems, considering both the phases before the transition and the modulated structures (see Fig. 2 for the $\text{Rb}_{0.3}\text{MoO}_3$ CDW phase). Our simulations, done using the SIESTA method, provide a clear understanding of the nature of the experimentally observed STM images, and solve the open questions in the interpretation of these images.

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Figures:

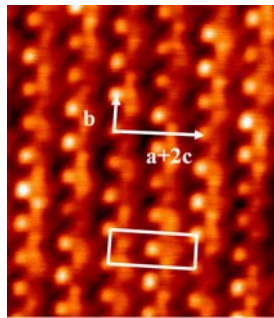


Fig 1. Constant Current mode topographical image of $6.2 \times 7.0 \text{ nm}^2$ on a (-201) plane of $\text{Rb}_{0.3}\text{MoO}_3$ at 63 K (bias voltage 420 mV, tunneling current 110 pA.)

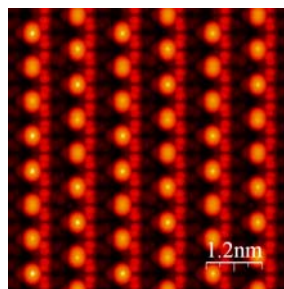


Figura 2. Theoretical image on the same plane of Fig. 1.

**SELF-ASSEMBLED MONOLAYERS OF PEPTIDE NUCLEIC ACIDS:
FROM THE MOLECULAR STRUCTURE TO BIOSENSOR APPLICATIONS.**

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Self-assembly and self-organization of molecules are the main strategies used in nature to permit life to emerge from its building blocks, and have inspired new trends in nanotechnology based on a bottom-up approach. Understanding the structure of molecular layers on surfaces is of a great importance because its atomic arrangement determines the mechanical properties, electronic behaviour and reactivity of surfaces. Therefore, the ability to control the surface structure at an atomic level is a crucial point for designing new type of biosensors more specific and highly sensitive.

Self-assembled monolayers (SAMs) of alkanethiols have been widely studied due to their relevant technological properties. Based on such knowledge, thiolated DNA has been immobilized on surfaces, although it usually forms disordered formless globular structures with reduced bioactivity, or requires the co-immobilization of spacer thiols in mixed monolayers. Peptide nucleic acid (PNA) is an achiral and uncharged DNA mimic of high biological and chemical stability. Therefore, we have investigated the interaction between single stranded PNA oligomers on metal surfaces. In spite of their remarkably length, up to 7 nm, cysteine-modified ssPNA oligomers assemble by themselves standing-up on gold surfaces similarly to the SAMs of short alkanethiols.

We present a thorough spectroscopic and morphological characterization of self assembled monolayers (SAMs) of thiol-derivatized PNA chains adsorbed on different kind of surfaces and nanoparticles. We look to correlate the structural properties of the layer with the biosensing activity. We have found that molecular orientation of PNAs strongly depends on surface coverage and the interaction with the substrate[1-3]. In the case of gold and for low coverage, PNA chains lie flat on the surface, while at high coverage PNA molecules realign their molecular axes with the surface normal to form partially ordered SAMs (Fig. 1). The change in the molecular orientation has been studied by Reflection Absorption Infrared Spectroscopy (RAIRS) and it has been confirmed by Atomic Force Microscopy (AFM) and X-ray absorption near-edge spectroscopy (XANES). A combination of the above mentioned techniques allow us to affirm that the structure of the SAMs is stabilized by molecule-molecule interactions through non-complementary nucleic bases of adjacent PNA molecules.

This molecular configuration is optimal for recognizing complementary ssDNA, and their specificity is such that they allow for discriminating even a point mutation in target ssDNA.

Self-assembly of ssPNA on other substrates, as pyrite and silicon, takes place with a different molecular structure, which is, again, directly related with the biosensing efficiency. These findings suggest interesting connotations both from a fundamental point of view (understanding self-assembly) and for the development of optimized biosensors.

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Figures:

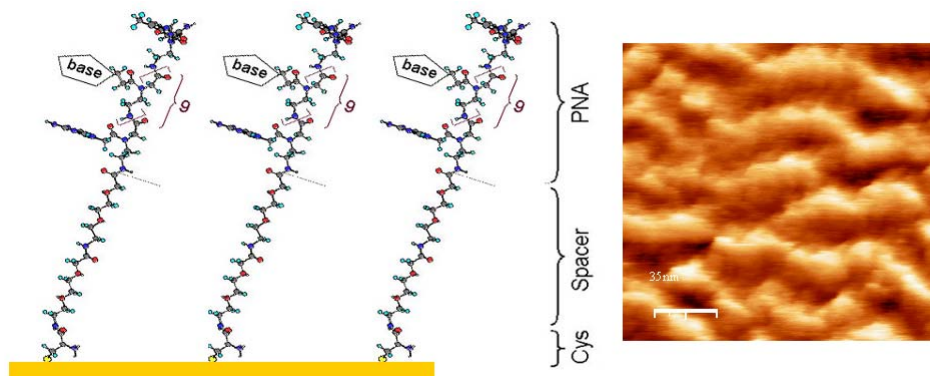


Figure1. Schematic model of SAMs of ssPNA on gold surface. AFM image showing PNA molecules standing-up on the surface.

**INTERFACIAL MAGNETISM IN ZNO/MNO₂ AND ZNO/CO₂O₃ THIN FILMS AND
MULTILAYERS**

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Although diluted magnetic semiconductors (DMSs) and carrier induced ferromagnetism are attracting considerable attention because of the possibility of incorporating magnetic degrees of freedom in traditional semiconductor materials¹ the origin of magnetism in the ZnO/MnO₂ and ZnO/Co₂O₃ systems is still not clear.

Since the recent theoretical prediction by Dietl *et al.*² of Curie temperatures above room temperature (RT FM) in the ZnO and the GaN systems containing 5% of Mn, several experimental studies have reported ferromagnetic like behaviour in these compounds³. Several theories exist about the mechanism responsible for ferromagnetism. In order to clarify if ferromagnetism is due to an interfacial effect or to the formation of a doped ZnO material thin film and multilayers of XO-ZnO (with different X=Mn or X=Co content) have been grown by pulse laser deposition (PLD) and characterized structurally, electrically and magnetically. The structural analysis is performed using X-ray diffraction, X-ray photoelectron spectroscopy and Raman spectroscopy techniques. Electrical characterization is carried out by Hall Effect measurements and magnetic characterization is studied with SQUID magnetometry. The origin of the ferromagnetic phase is unambiguously determined to be due to the presence of mixed-valence state in both Mn and Co oxides at the diffusion front of Zn into the Mn or Co oxide grains. In order to clarify that particular aspect multilayer of ZnO/MnO₂ and ZnO/Co₃O₄ were grown and characterized. The measured magnetization was 2 orders of magnitude larger than that of the bulk. This means that magnetism in these systems is due to interfaces.

This mechanism explains the origin of the room temperature magnetism and anticipates a unique and promising material for spintronic devices.

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CARBON NANOTUBES: TOWARDS TECHNOLOGICAL APPLICATIONS

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Carbon nanotubes (CNTs) are a new class of nanoscale objects with exceptional properties. [1] Their nanometer size, their high aspect ratio, their low specific weight, their superior mechanical properties (tensile modulus of 1 TPa, tensile strength of 200 MPa), their electronic characteristics (ranging from insulator to metal), and their thermal behavior renders this class of materials of high interest for applications in various areas of technology [2]. These range from nanoelectronic devices, flat panel screens, microscopy probes as well as energy storage media (batteries, fuel cells). Further promising applications can be expected from the development of new classes of advanced composite materials with improved structural or/and functional characteristics. This bears new options for reinforced plastics, and engineered polymers with superior electrical/thermal/opto-electronical properties [3,4]. Here, CNT-based products will largely impact on the rapidly growing market for novel high-performance nanostructured materials.

This presentation will give an overview of the basics of carbon nanotubes (structure and properties) and then focus especially onto the field of applications. Examples in various areas of technological interest will underline the high application potential of these nanoscale objects. Bottlenecks to be overcome for industrial use such as issues related to mass-production, processing, assembly, and interactions, will be discussed.

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GENESIS RED

Spanish Nanoelectronics and Smart Systems Integration Platform

GENESIS RED is the Spanish Nanoelectronics and Smart Systems Integration Platform (www.genesisred.net). GENESIS RED puts together Spanish industries, research centres and universities from the electronics, informatics and telecommunications sectors. GENESIS RED is supported by the Spanish Government through the Centre for Industrial Technology Development (CDTI), the Ministry of Education and Science (MEC) and the Ministry of Industry, Tourism and Trade (MITyC). The main goal of GENESIS RED is to strengthen the position of the Spanish scientific and industrial community towards the 7th Framework Programme. For this purpose, GENESIS RED has the next functions:

- To act as “unique window” and mirror group for the European Platforms ENIAC (European Nanoelectronics Initiative Advisory Council) and EPoSSI (European Technology Platform on Smart Systems Integration).
- To elaborate a map of capabilities and potentialities in order to establish recommendations concerning strategic research lines in the Nanoelectronics and Smart System Integration fields.
- To improve the participation of the Spanish organizations in the preparative actions of the 7th Framework Programme, being active in the new instruments such as Platforms and Join Technology Initiatives (JTIs).
- To improve the collaboration within the Spanish Nanoelectronics Community.
- To collaborate with the public institutions to identify the main areas of industrial innovation and scientific excellence.

Genesis Red has set-up a Scientific Committee who is drawing up a report focused on the state of Nanoelectronics in Spain in order to establish the areas where Spanish competences and expertises are well positioned at European level. GENESIS RED has divided its technical activity in 9 priorities:

- More Moore
- Beyond CMOS
- More than Moore
- Heterogeneous Integration
- Design Automation
- Equipment and Materials
- Training
- Infrastructures
- Smart Systems Integration

GENESIS RED has been promoted by GAIA- Asociación de Industrias de las Tecnologías Electrónicas y de la Información del País Vasco, CNM- Centro Nacional de Microelectrónica and CIDETEC- Centro de Tecnologías Electroquímicas.



CHARGE TRANSPORT PROPERTIES OF DONOR-ACCEPTOR ORGANIC RADICALS AND SELF ASSEMBLED ORGANIC MONOLAYERS

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Systems formed by donor and acceptor units covalently attached by an organic bridge are of both scientific and industrial interest for the investigation of Intramolecular Electron Transfer (IET) phenomena. The interest arises from the potential use of such systems as molecular wires on integrated molecular-sized devices [1] such as photo-optical, photoconductors, nonlinear Optics, telecommunications, informatics' storage or even lasers devices. From the theoretical point of view, these studies could allow the rules for the prediction and control of electron propagation in molecular wires to be worked out [2].

We will study the intramolecular electron transfer phenomena of two neutral paramagnetic donor-acceptor dyads based on a polychlorinated triphenylmethyl radical acceptor unit and a ferrocene linked by an vinylene π - bridging unit (Fig.1a). These family of compounds present interesting optical, magnetic and electronic properties like non linear optical properties [3] or supramolecular photomagnetism [4] and they can also act as molecular electrochemical switches [5]. These compounds exhibit broad absorptions situated in the near IR region with band maxima around 1500 nm which are associated with the intramolecular charge transfer. The energy of this intramolecular electron transfer can be tuned by changing solvent. Solvent dependence was investigated in 22 different solvents revealing positive solvatochromic shifts of the peak maxima to lower energy with increasing the solvent polarity (Fig.1b). Cyclic voltammetry of the compounds show reversible one electron redox processes associated with the oxidation of the ferrocene and reduction of the polychlorotriphenylmethyl radical subunits, respectively. The solvent dependence of the redox potentials has been investigated electrochemically in different solvents and a shift from Marcus- *normal*- to *inverted* region with the solvent polarity is found. As far as we know these are the first molecular systems where it is possible to pass from normal to inverted Marcus region simply by changing the polarity of the solvent.

The final interest of these systems is its potential use as molecular wires in integrated devices. For this reason we need to explore the electronic factors affecting electrical transport of molecules in metal-molecule-metal junctions. In applications where a number of molecules have to be addressed as an ensemble, complex molecule-substrate, intermolecular interactions and deformation of molecules would affect the self-assembly influencing their collective behavior and hence the electronic transport through them. The use of AFM with conducting tips provides the ability to vary the load on the nano-contact and also opens the way for exploring electron transfer as a function of molecular deformation (Fig. 2). Results on the influence of mechanical stress on the structural and electrical properties of self-assembled alkylthiols on gold surfaces as a function of the tip pressure will be also presented.

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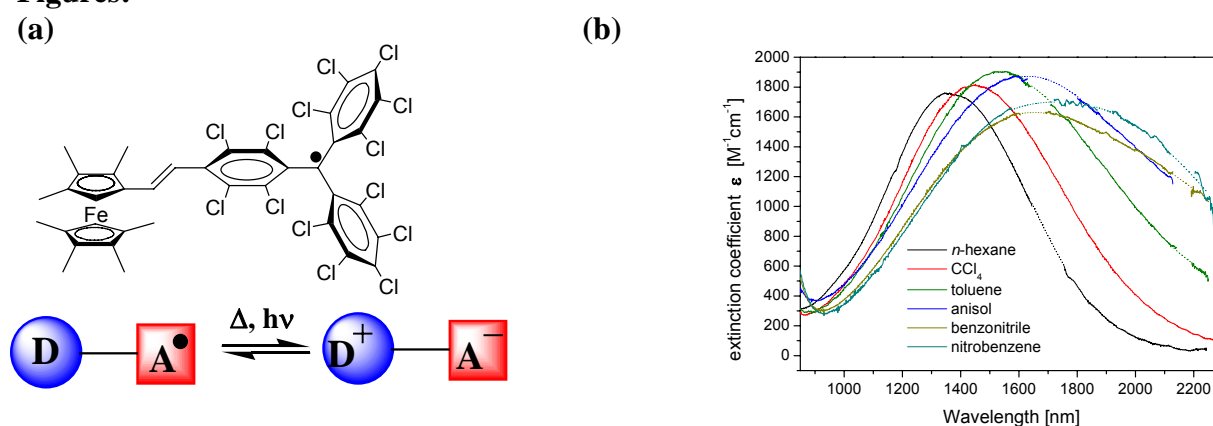


Figure 1. (a) Scheme of the Intramolecular electron transfer process in our Donor-Acceptor organic radical. (b) Intramolecular electron transfer band in various solvents.

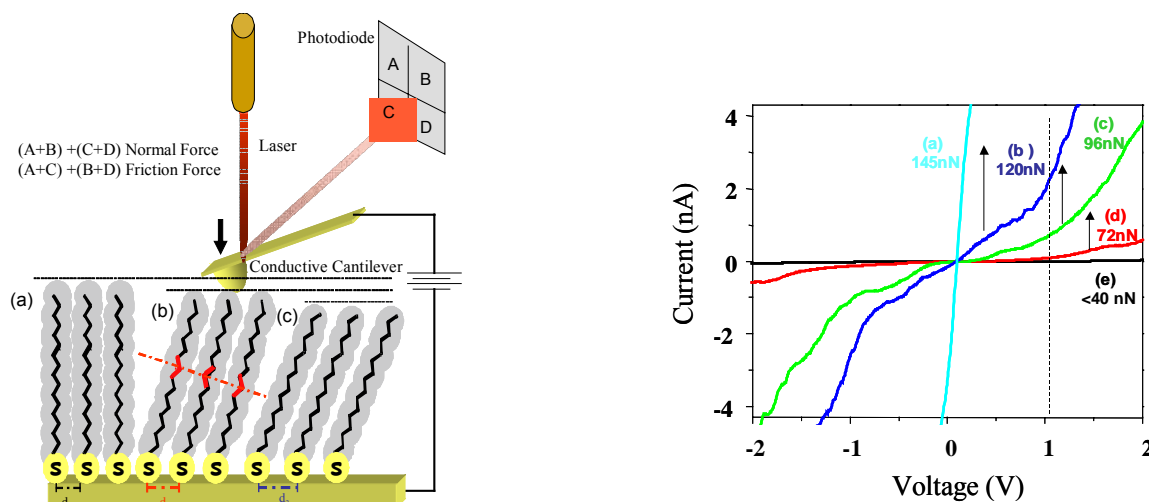


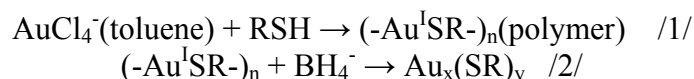
Figure 2. (a) Conducting AFM used to probe the charge transport properties of self assembled monolayer at various applied load. (b) Current-voltage (I-V) characteristics for a $\text{CH}_3(\text{CH}_2)_{15}\text{SH}$ monolayer junction as a function of applied load on the conducting tip.

Microstructure and magnetic behaviour of alkanethiol-capped gold nanoparticles.

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Metallic nanoparticles (NPs) are extensively studied since they exhibit novel electronic, optical and magnetic properties. In particular, the study of magnetism in clusters of palladium and gold has attracted special attention as these elements are non-magnetic in bulk. Alkanethiol derivatised gold NPs [1], as well as self-assembled alkanethiol monolayers on gold surfaces [2], have shown a permanent magnetism that it is at the present moment partially understood [3]. In the present paper we show some new results in relation to the microstructure and magnetic behaviour of the alkanethiol capped gold NPs.

The alkanethiolate-capped gold NPs have been obtained by a liquid-liquid phase reduction at room temperature, based on the Brust method [4]. This method is a two-step process described as follows:



In the first step Au(III) is reduced to Au(I) by oxidizing the thiols to disulfides. In non polar solvents the Au(I)(SR) species aggregate forming a polymeric phase. In the second step the addition of sodium borohydride leads to the reduction of all gold species to form the gold clusters surrounded by thiolates. In the present work we have isolated the intermediate Au(I)-SR(polymer) phase as well as the Au-SR NPs. The microstructure and the magnetic properties have been investigated for the two samples.

Figure 1 shows the corresponding TEM micrographs. The Au-SR sample is constituted by well defined spherical-like NPs with an average particle diameter of 2.0 nm. The intermediate Au(I)-SR(polymer) phase is an amorphous like sample difficult to study by TEM due to the fact that under electron beam irradiation evolves with formation of nanoparticles. Chemical analysis shows Au:S atomic ratios of 1 and 1.7 respectively for the Au(I)-SR(polymer) and Au-SR samples.

The magnetic study shown in Figure 2 clearly shows that the addition of a reduction agent is necessary to obtain the anomalous ferromagnetic-like behaviour previously described for the Au-SR systems (either gold NPs or gold films functionalised with alkane-thiols). The Au-SR samples shows saturation magnetisation values of 0.095 emu/g of Au and coercive fields of 180 Oe at 5K. It has been previously proposed [4,5] that in thiol-capped gold NPs, small Au:S atomic ratios, charge transfer from Au 5d to S 3p and small sizes of the NPs are necessary to produce a 5d density of holes in the gold atoms leading to the strong anisotropy and the observed permanent magnetism. The present work shows that the Au(I)-SR(polymer) sample corresponds to the maximum of Au to S charge transfer, the minimum Au:S atomic ratios and an extreme reduction of particle size by complete dispersion of the gold atoms in the alkanethiol phase. However the situation is not the one producing the permanent magnetic moment as clearly shown in Figure 2. An intermediate state between Au(I) and metallic gold seems to be in the origin of this behaviour. The X-Ray Absorption spectroscopy (XAS) at the Au LIII and Au LII edges is providing a complete analysis of the atomic and electronic structure necessary to understand the singular magnetic behaviour.

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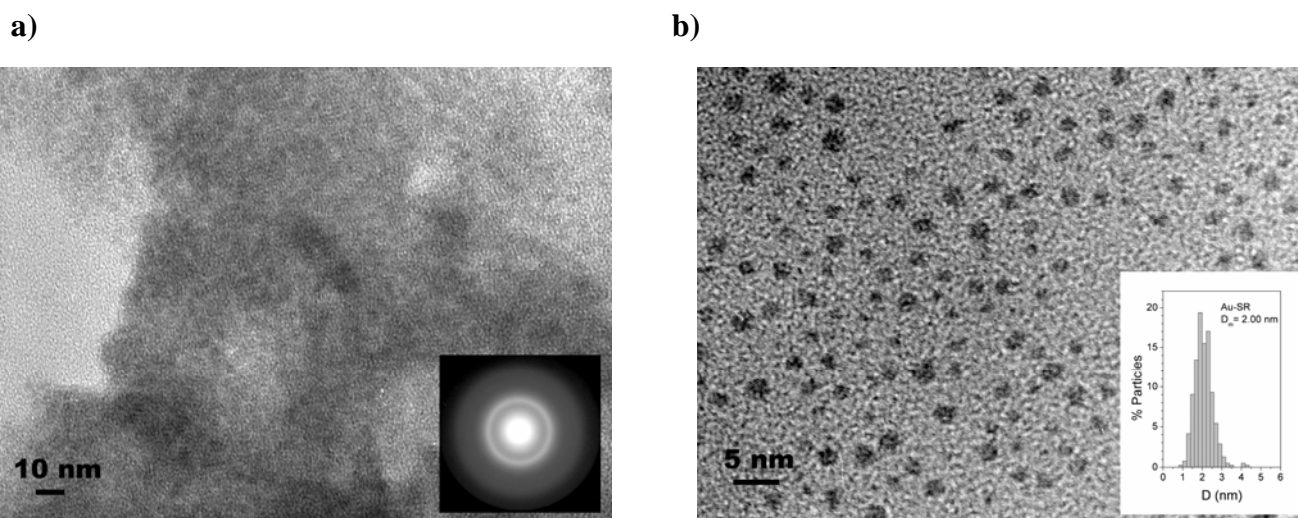


Figure 1. (a) TEM micrograph and the corresponding selected area electron diffraction (SAED) patterns of Au(I)-SR(polymer). (b) TEM micrograph and particle size distribution histogram of the Au-SR capped nanoparticles.

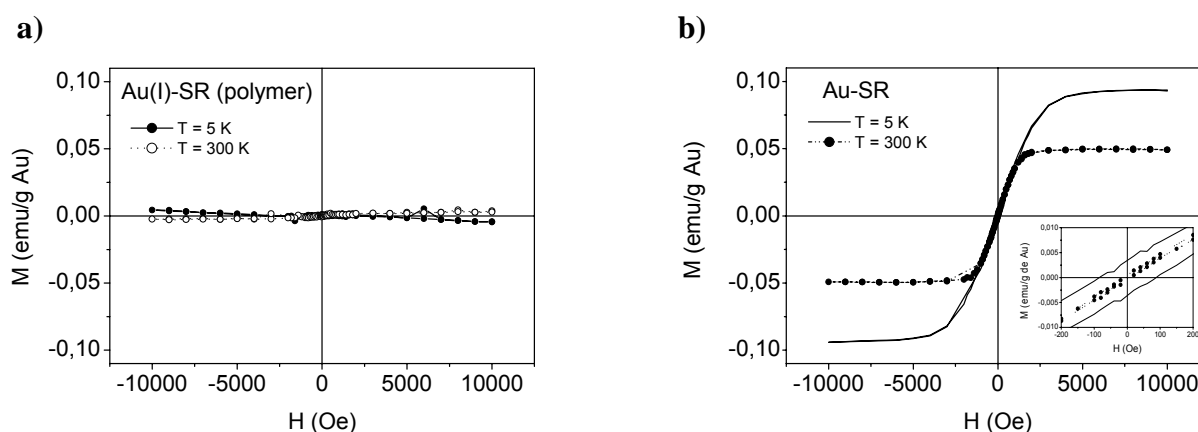


Figure 2. Hysteresis loops corresponding to the intermediate Au(I)-SR(polymer) precursor (a) and the gold thiol-capped nanoparticles Au-SR (b), at 5 and 300 K.

AC IMPEDANCE SPECTROSCOPY OF INDIVIDUAL TIN-OXIDE CONTACTED USING DUAL BEAM FIB NANOLITHOGRAPHY

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The measurement of the electrical properties of individual 1D-nanostructures is still a challenging issue due to the complex problems related to the fabrication of electrical nanocontacts with nanoprecision, in a controlled way, as well as, to the understanding of the involved contact physic mechanisms that can introduce higher contact resistance than the nanowire itself. In this work, a systematic procedure to overcome these difficulties and go in deep in the nanocontact physics is presented.

Individual tin-oxide (SnO₂) nanowires (NWs) -synthesized in a chemical vapour growth at low temperatures (550-750°C), by the gas phase decomposition of a molecular precursor [Sn(OtBu)₄] following a method explained elsewhere²-, have been contacted using a platinum (Pt) nanolithography process with help of a Dual Beam FIB, designed to reduce the damage and modification of the contacted NWs during the nanofabrication process³.

The electrical response of these bottom-up devices based on one single NW have been studied performing 2- and 4-probe DC measurements, enabling the estimation of the SnO₂ NWs resistivities and Pt-NW contact resistances. Moreover, the dependence of these electrical parameters as function of temperature (T) has also been evaluated.

AC Impedance Spectroscopy is a powerful technique suitable to study the different electrical charge transport mechanisms which can take place inside solid materials, and it can be considered as a good characterization technique to reach a better understanding of the electrical transport existing inside 1D-nanomaterials and nanostructures.

AC Impedance Spectroscopy has been applied to some of these bottom-up devices allowing the development of both an equivalent circuit and the study of the frequency response of Pt-SnO₂ NW junctions, which are known to be Schottky rectifying contacts. A full characterisation of these FIB-fabricated contacts is required to improve their quality, and the capabilities of future bottom-up nanodevices.

To our knowledge, these are the first attempts of using AC impedance spectroscopy to characterise a device based on a single nanowire.

Finally, the possibility of using these nanodevices and AC Impedance measurements to detect different gases will be discussed.

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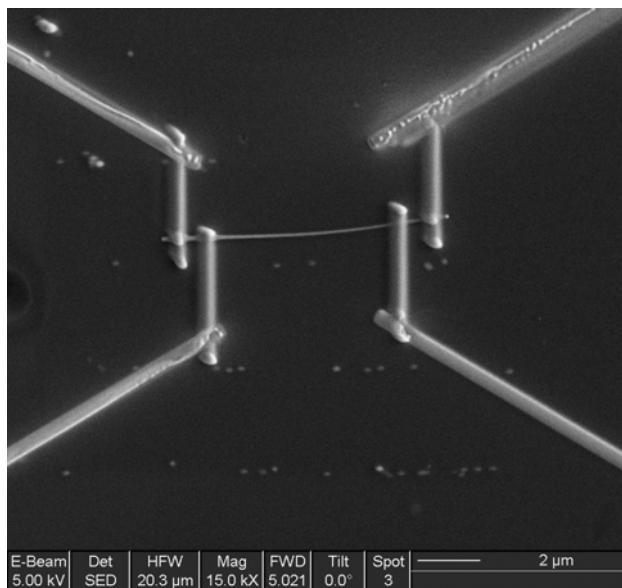


Fig.1. SnO₂ NW contacted in 4-probe configuration using a Pt-nanolithography process with help of a Dual Beam FIB

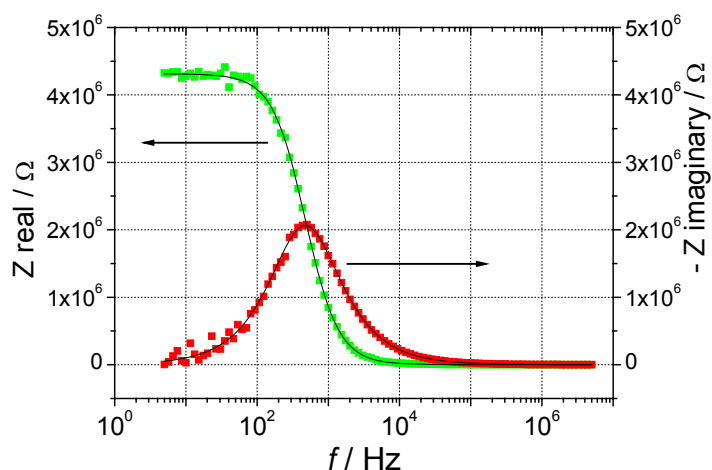


Fig.2. Z real and Z imaginary frequency response of a single SnO₂ NW. The measured data (points) are fitted to an equivalent circuit response (line).

“MODELLING FOR NANOTECHNOLOGY” - M4NANO INITIATIVE

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“Modelling for Nanotechnology” (M4nano) is a WEB-based initiative led by four Spanish Institutions: Phantoms Foundation, Parque Científico de Madrid (PCM), Universidad Autónoma de Madrid (UAM) and Universidad Complutense to maintain a systematic flow of information among research groups and therefore avoid that research efforts in Nanomodelling remain fragmented.

Networking is vital to any scientist and even more so for persons working in the interdisciplinary field of Nanotechnology and in particular Nanomodelling. To fulfil this necessity, M4nano will provide a comprehensive guide -“who’s who”- of groups working in Modelling at the nanoscale listing their accomplishments, background, infrastructures, projects and publications. In this way, M4Nano completes the aim of both raising awareness of scientists in Nanotechnology modelling issues and aiding them in developing beneficial collaborations and employment opportunities.

Emerging research areas such as Molecular Electronics, Biotechnology, Nanophotonics, Nanofluidics or Quantum Computing could lead in the mid-term future to possible elements of nano-based devices. Modelling behaviour of these possible nanodevices is therefore becoming more and more important and should allow to: (i) Visualise what happens inside a device (ii) Optimise the devices under study (iii) Improve understanding of device properties (physical, chemical, etc.).

M4nano in close collaboration with other European Research Institutions deeply involved in “modelling at the nanoscale” will develop tools such as a user’s database, a forum to stimulate discussions about the future of Nanocomputing, a source of documents (courses, seminars, etc.) on modelling issues, etc. and in the mid-term future implement a computational HUB, repository of simulation codes useful for modelling and design of nanoscale electronic devices.

Information spreading will also be enhanced using mailing list alerts, press releases and flyers. Collaborations with similar initiatives such as the NanoHub (USA) or Icode (Italy) will also be set-up.

WEB site: <http://www.m4nano.com>

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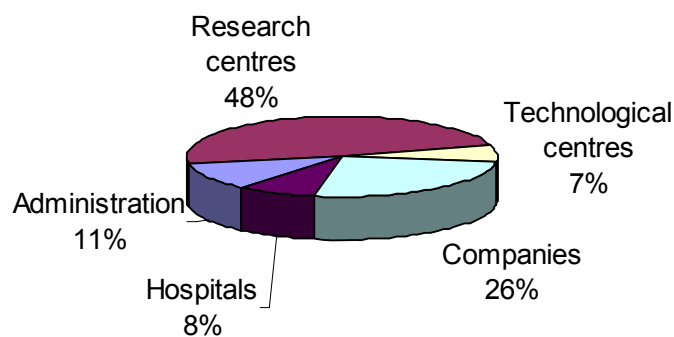
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SPANISH NANOMEDICINE PLATFORM

The **Spanish NanoMedicine Platform (SNMP)** is an initiative of industries and research centres applying nanotechnologies for medical applications, supported by the Spanish government through the Centre for Industrial Technology Development (CDTI), in the context of the “nanotechnology action” of the Spanish Ministry of Education and Science (MEC), Ministry of Industry, Tourism and Trade (MICyT) and Ministry of Health. More than 70 groups are actually members of the Platform.

Participation in the Spanish Platform on Nanomedicine



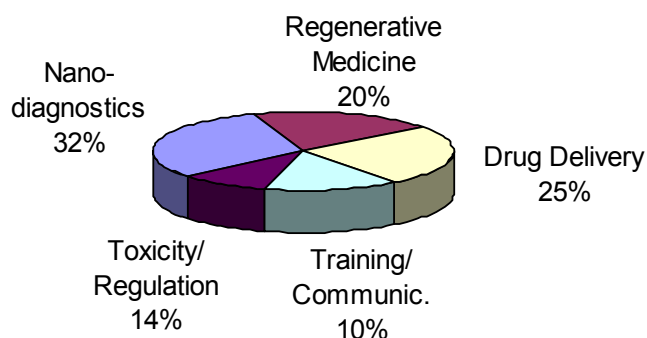
The policy objectives of the Spanish NanoMedicine Platform are:

- Set-up a “unique window” for the Nanomedicine community in Spain,
- Improve the collaboration of the Spanish Nanomedicine community in international initiatives, from transnational cooperations to European projects, especially regarding the establishment of the European Technology Platforms,
- Establish recommendations concerning strategic research lines in the Nanomedicine field,
- Act as a community regarding the whole society concerning Nanomedicine aspects.

The Spanish NanoMedicine Platform has divided its activity in five strategic priorities:

- 1- Nanodiagnostics
- 2- Regenerative Medicine
- 3- Drug Delivery
- 4- Toxicity and Regulation
- 5- Training and Communication

Participation in the Working Groups



Each working group is drawing up a report focused on the state of Nanomedicine in Spain in order to establish the areas where Spanish competences and expertise are well positioned at European level. The objective of those papers is also to open recommendations to the Spanish government which aim is to strongly support Nanomedicine initiatives.

RESONANT CHARGE TRANSFER AT SURFACES: AN AB INITIO APPROACH

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I will present a scheme for the calculation of the resonant charge-transfer rates of electrons from adsorbates to metallic substrates. The electrons initially reside in electronic excited states in the adsorbates. Our calculations are based on first-principles density-functional calculations of the combined adsorbate-substrate system using finite slabs. These results are then combined with bulk calculations of the substrate material to obtain the Green's function of the semi-infinite system. Our results are thus based on a realistic description of the electronic structure of both systems, the substrate and the adsorbate, and the interaction between them. This scheme has also been applied recently to the calculation of the elastic width of quantum well states at alkali overlayers on Cu(111) [1]. We focus here in two cases: i) the c(4x2)-S/Ru(0001) surface [2], and ii) Ar monolayers on Ru(0001) [3]. In the first case we find a charge transfer time well below the femtosecond scale, in very good agreement with the experimental measurements based on core-hole-spectroscopy using Coster-Kronig decay channels. We also predict the variation of the observed charge transfer time with the polarization of the excitation light (see the figure). This effect still waits for experimental confirmation. For the case of Ar on Ru our calculated values and trends are in also good agreement with experiment.

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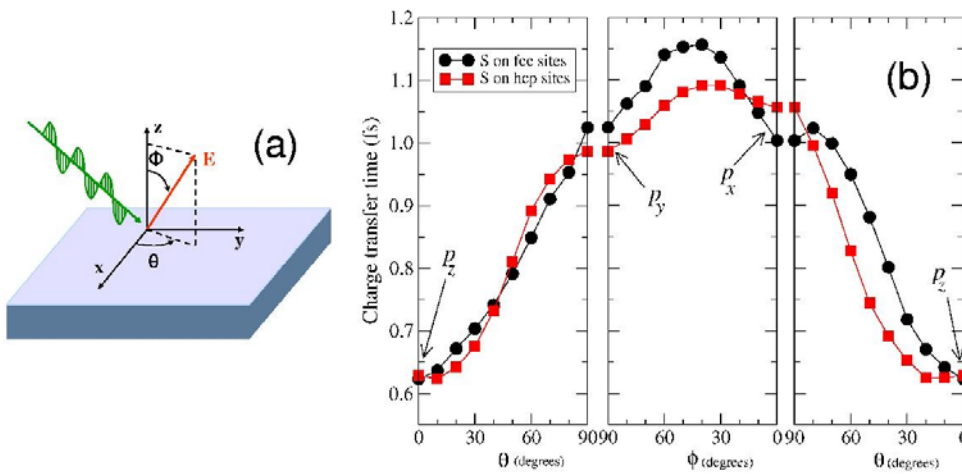


Figure. Charge transfer time in the c(4x2)-S/Ru(0001) surface as a function of the direction of the electric field in the experiment (see the scheme in panel (a)). Different excitation geometries translate to different initial electronic wavepackets. The wavepackets are constructed by projecting linear combinations of the sulfur 3p states onto the energy window corresponding to the resonance studied in Ref. [2]. The charge-transfer time is then obtained from the evolution of the survival amplitude of those wavepackets.

DEVELOPMENT OF NANOMECHANICAL BIOCHIPS FOR FUNCTIONAL GENOMICS AND PROTEOMICS

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Nanomechanical biosensors have emerged as a promising platform for specific biological detection. The operation principle is that molecular recognition on the surface of a microcantilever produces a deflection of few nanometers (DC detection) and a shift of the resonant frequency of few Hz (AC-Detection) [1-3]. Among the advantages of these biosensors are direct detection without need of labeling with fluorescent or radioactive molecules, very high sensitivity, small sensor area, and suitability for further integration using CMOS silicon technology [4]. Applications include detection of nucleic acids, proteins and pathogens. Here, we present several developments addressed to obtain a nanomechanical biochip for functional genomics and proteomics. These developments include: a) Fabrication of cantilevers in the novel polymer SU-8, ii) Development of a new optical readout technique of cantilever arrays and iii) Optical actuation of cantilever and Q-enhancement via a feedback amplifier.

Firstly, we present a technology for the fabrication of cantilever arrays aimed to develop an integrated biosensor microsystem. The fabrication process is based on spin coating of the photosensitive polymer and near-ultraviolet exposure. Arrays of up to 33 microcantilevers are fabricated in the novel polymer material SU-8. The low Young's modulus of the polymer, 40 times lower than that of silicon, enables to improve the sensitivity of the sensor device for target detection. The devices exhibit high sensitivity for detection of the biomolecular interactions biotin/avidin, for specific detection of the human growth hormone and for detection of DNA [5, 6].

For readout of the microcantilever arrays a new optical technique has been developed [7]. This combines the optical beam deflection technique and the scanning of the incident laser beam by using a voice-coil actuator. The individual motion of each microcantilever is obtained by correlation of the total photocurrent collected in a photodetector array, the position of the laser beam and the coordinates of the laser spot centroid on the photodetector. The technique provides sub-angstrom resolution in the cantilever deflection and it allows the readout of tens of cantilevers per second. It is demonstrated that the combination of the optical sequential readout and the use of passive cantilevers acting as reference to remove non specific signals, such as small temperature, pH and ionic strength variations, enhances the sensitivity by more than one order of magnitude. Examples will be shown of specific detection of DNA sequences. In addition, by implementing a two-dimensional scanning system the profiles of the cantilevers are obtained in real-time, i.e., during the adsorption of biomolecules [8].

Finally, a major development of biological sensors based on nanomechanical resonators requires of new developments in actuation and transduction techniques compatible with measurements in aqueous environments. Here we present new experimental and theoretical results for optimum optical excitation of different vibration modes in liquid [9]. The experiments show how the vibration of the first three vibration modes depends on the position of the intensity modulated laser beam along the cantilever. The experimental results are supported by a theoretical model. In addition, we discuss the implications of the Q-control

enhancement in the signal and noise of the vibration response [10]. These developments are applied for detection of bacteria.

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TEACHING QUANTUM NANOMAGNETISM

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The origin of magnetism is quantum and its founding fathers were capable to explain the change in the coulomb interaction between two electrons when their spins were coupled to states having total spin $S=1$ and $S=0$. The case is that this quantum vision of magnetism can not explain the magnetic properties of macroscopic systems. This is because processes observed on the macroscopic scales result from weak interactions unaccounted for in simple quantum models. This is the reason why most of the works performed on magnetism during the last century have been based upon classical theories. That is, the practical question of how a piece of iron magnetizes in an applied magnetic field has nothing to do with quantum Hamiltonians. The interactions we have to consider in these cases are the magnetic anisotropy owing to the symmetry of the crystal, the magnetic dipole interaction that breaks the magnet into domains, interactions of domain walls with defects, impurities, itinerant electrons, etc.

The trend of new technologies to reduce the size of the fabricated objects has been made possible the emergency of new magnetic systems which may be considered as nanocompasses. The case is that the total magnetic moment of a magnetic entity formed by several tens of atoms satisfies the quantum commutation relation $M_i - M_j = 2i\mu_B\epsilon_{ijk} M_k$ indicating that it entitled “Lectures on Magnetism “ will not be possible to determine the orientation of its three components with high accuracy by macroscopic measurements. The study of both the frontier and overlapping between the classical and quantum worlds can be approached in magnetism in different ways. Molecular magnets are between many different systems the best candidates to perform such studies because the knowledge of their spin Hamiltonian allows to get one to one correlation between theory and experimental results.

This new book we have written entitled “Lectures on Magnetism (with 128 Problems) is divided into three chapters depending on the dimensions of the magnetic object. The first chapter deals with the magnetism of individual spins at the nanometer scale, the second explains the magnetic order appearing at the mesoscopic scale and the third chapter explains the magnetic properties of macroscopic magnets. That is, we incorporate, for the first time in a book the teaching of quantum properties of nanomagnets. For example, we first explain the origin of both magnetic exchange and magnetic anisotropy in a microscopic volume and the superparamagnetic properties of such magnets. In the absence of magnetic external fields the two possible orientations of the magnetic moment along the easy axis are separated by the barrier height associated to the magnetic anisotropy which is fully determined by the parameters entering the spin Hamiltonian. We also discuss under which circumstances it is possible to observe the quantum behaviour of the total magnetic moment of these microscopic volumes by discussing the cases associated to different spin Hamiltonians. To address such problems we have considered the case of the spin-phonon interaction and the calculation of the quantum tunnelling splitting, Δ , associated to the overlapping of the spin wave functions of states separated by an energy barrier. The fraction, P , of spins tunneling

through the anisotropy barrier depends on how strong is the overlapping of the wave functions of the spin states in resonance at the two sides of the barrier and on the sweep rate of the magnetic field, α : $P = 1 - \exp(-\pi\Delta^2/2\alpha)$. We have also explained the so called quantum magnetization curve and how it does depend on the parameters of the spin Hamiltonian and on both the longitudinal and transversal magnetic fields and on their corresponding sweeping rates. It is also carefully studied the case of the dependence of Δ on the transversal magnetic field which has been used to explain the interference effects associated to the two possible least-action tunnelling paths for the spin reversal. The modelling of the spin-phonon interaction has been also used to explain both the emission of photons and phonons in the demagnetization process of these nanomagnets.

Summarising I will introduce to the audience a new text book which explains at the student level the most innovative aspects of the quantum properties of nanomagnets.

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2.- NEW BOOK:

**LECTURES ON MAGNETISM (with 128 Problems)
Eugene Chudnovsky and Javier Tejada
RINTON PRESS 2006. Princeton (2006).**

Electrostatic manipulation of gold nanoparticles using an atomic force microscope.

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There exist tools such as Atomic Force Microscopy (AFM), Scanning Tunneling Microscopy (STM), and Scanning Electron Microscopy (SEM) [1]-[2] that enable to manipulate elements of nanometer sizes. In the present case, we investigate the electrostatic nanomanipulation with AFM

Initial attempts at manipulation of nanoparticles with the AFM were based on pushing the nanoparticle with the AFM tip [2] [3] [4] [5]. Unfortunately, the pushing process does not enable building 3D structures. We will show that the electrostatic manipulation overcome these difficulties.

Electrostatic nanomanipulation uses electrostatic forces to detach the particle from the substrate and Van der Waals forces [6] to attach back the particle to the substrate, or viceversa. The election of one procedure or another depends on the relative value of the Van der Waals forces of the particle-substrate and particle-tip systems. In both cases, during the translation process, the nanoparticle remains adhered on the tip.

To perform the electrostatic manipulation [7] the tip must be situated at a fixed distance on the nanoparticle. When a potential difference is applied between the AFM tip and the substrate, the generated electrostatic field exercises a force on the nanoparticle enabling to detach the particle from the substrate.

The manipulation method requires a precise control of the tip. If the tip is too far from the nanoparticle the transfer does not occur. On the other hand, if the tip is too near to the particle, the tip collapses onto the nanoparticle on the substrate surface [8] [9]. It is necessary to take into account the deflection of the cantilever when the potential is applied. Simulations estimate this deflection to be about 3 nm for 10 V applied. With this potential the maximum tip-nanoparticle distance is 20 nm (see fig. 1). In this case the tip-particle distance before applying the potential must be approximately 23 nm.

In Fig. 2a and 2b we show the transport of a gold nanoparticle from position A to position B performed electrostatically.

A graph of the deflection signal as a function of time during the nanomanipulation experiment is shown in Fig. 3. The protocol is (1) push the tip onto the nanoparticle (2) raise the piezo 50 nm (3) apply 10V during 6 seconds. Nothing is happening, so (4) approach the piezo 5 nm to the nanoparticle (5) apply 10V during 6 seconds. Nothing is happening, so (6) approach the piezo 5 nm to the nanoparticle (7) apply 10V during 6 seconds. There are a change in AFM deflection so (8) raise the piezo 100 nm (9) move the piezo horizontally (10) switch on the feedback.

To create 3D structures accurately we need to transport one particle over other particles and deposit it with precision, otherwise, we can destroy the structure. The images in figure 4 show the possibility of positioning a nanoparticle on others by means of electrostatic manipulation.

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Figures:

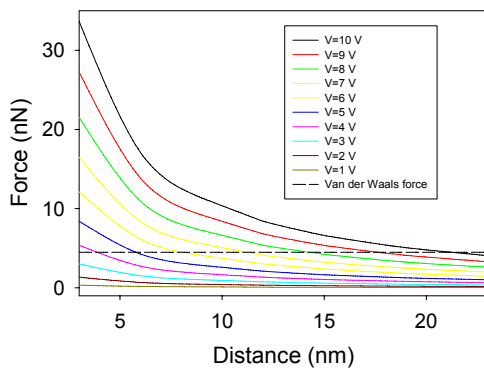


Figure 1: Force on the nanoparticle versus tip-nanoparticle distance for different applied potentials. The discontinuous black line is the Van der Waals force between the particle and the substrate. At 10V the transfer of the particle occurs at approximately 20 nm tip-particle distance.

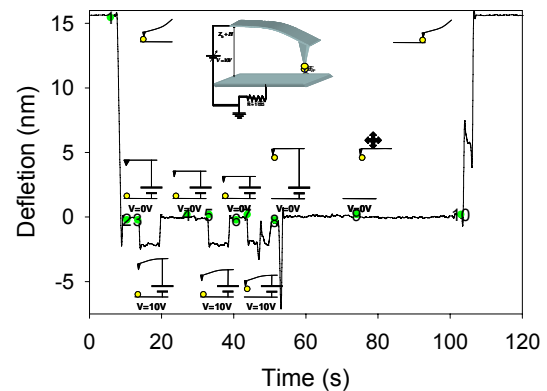


Figure 3: Deflection signal as a function of time during the nanomanipulation.

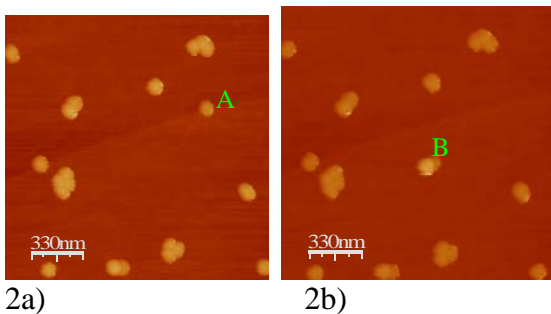


Figure 2: 2a and 2b we show the transport of a gold nanoparticle from position A to position B performed electrostatically.

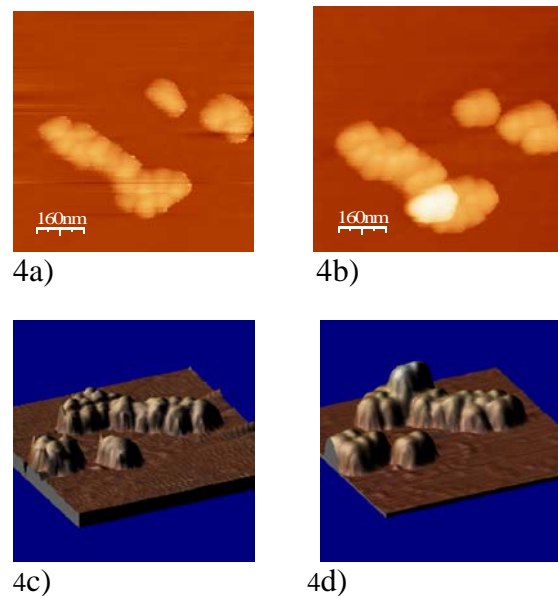


Figure 4: (a) and (b) 2D AFM images before and after the deposition of a nanoparticle on an aggregation of nanoparticles. (c) and (d) the corresponding 3D images before and after the deposition.

ABOUT THE STRATEGIC ACTION ON NANOSCIENCE AND NANOTECHNOLOGY

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Along the last decade, the scientific and technological advances have enabled the fabrication, tailoring and manipulation of matter in a controlled way at a nanometric scale, that have switched on new advanced research and developments. While both bottom-up and top-down routes are currently proposed, investigations at the nanoscale present a clear interdisciplinary character that requires the involvement of researchers with complementary expertise. In this way, new branches of science and technology are emerging involving physicists, chemists, biologists or materials engineers, among others. The knowledge so acquired, makes one to foresee an unprecedented understanding and control of matter offering new opportunities to various industrial sectors as for example in biomedicine and pharmacy, electronics, energy and environment, metallurgy, telecommunications, advanced equipments or computation and information storage.

Within this scenario, the Ministry of Science and Education, according to the planning established in the National Plans of Research, Development and Innovation for the periode 2004-2007 launched an specific Strategic Action on Nanoscience and Nanotechnology to promote scientific and technological research in that area. A first extraordinary call for projects was opened with an aim to fund innovative projects of scientific excellence and finalist trend incorporating groups of complementary disciplines in the “nanoworld”.

In this presentation, a summary of final statistics is introduced that concerns applied and funded projects as well as thematic areas, geographical and research centres distributions. In addition, specific scientific and technological areas with potential interest have been identified. Finally, information will be given on current alternative international programs on nanoscience and nanotechnology.

Nanochemistry Platform

Jaume Veciana

Institut de Ciència de Materials de Barcelona (CSIC)

As chemistry is an enabling science, research into the fundamentals of Nanoscience and applications derived from Nanotechnology will give the European research area and consequently the European Union the edge over its global competitors. In the field of Nanoscience and Nanotechnology, the work and research being conducted to date is (still) largely empirical and, therefore, there is a great need to develop the fundamental understanding and knowledge associated with working at the nanoscale. Nanoscience provides an understanding of a nano-object (material, particle, etc.) with its environment. The major challenge facing academics is to be able to predict the change in any (material) property when changing the size scale from above 100 nm to below 10 nm. At present the contemporary understanding of Nanoscience is used to enhance existing materials and products, but in the future it will lead to new interesting products by design. Nanoscience is a disruptive, out-of-the-box discipline, but nonetheless a key-enabler, leading to innovation, growth and a better quality of life as well as more competitiveness. Industry can and should consider Nanoscience and its related Nanotechnologies as an innovation toolkit, which can lead to new materials at the nanoscale, which spawn new products and ideas for the market and assist in creating up-and-coming markets.

In order to boost chemical research, development and innovation activities related, among others, with Nanoscience and Nanotechnology it has been created the “*European Technology Platform for Sustainable Chemistry*”, named *SusChem* (www.suschem.org), as well as its Spanish homologous platform, called “*Plataforma Tecnológica Española de Química Sostenible*” (www.pte-quimicasostenible.org), *PETEQUUS*, which are supported by more than 30 European and National Chemical and Biochemical Industry Federations (CEFIC, FEIQUE, EUROPABIO, ASEBIO, etc.), private corporations and official institutions (European Commission DG Research, Ministerio de Educación y Ciencia, CDTI, etc.). Another important facet of both platforms is in the involvement of the public, governments and stakeholders in an open and transparent discussion addressed for the successful exploitation of Nanoscience and Nanotechnology, among others. To accomplish these targets *SusChem* has elaborated a Strategic Research Agenda which outlines the future priorities for European research efforts as perceived by its stakeholders. This document identifies key areas of research, limitations and hurdles faced by researchers proposing also amendments for future activities. The elaboration of such a document was conducted in an open and transparent fashion with participants from all spheres of society, from non-governmental agencies through academics to the industry representatives.

In this short presentation the structure and organization of *SusChem* and *PETEQUUS* as well as the most important aspects related with Nanoscience and Nanotechnology of their Strategic Research Agenda will be summarized.

Pamplona 20-23, March 2006



3rd NANOSPAIN WORKSHOP

WORKING GROUPS

1. **Molecular Electronics** (Coordinators: Julio Gomez & Pablo Ordejon)
2. **NanoBiotechnology** (Coordinator: Josep Samitier & Laura Lechuga)
3. **NanoEnergy** (Coordinators: J.R. Morante & Xavier Obradors)
4. **NanoFabrication** (Coordinators: Francesc Perez-Murano & Fernando Briones)
5. **Industrial** (Coordinators: Isabel Obieta & Emilio Prieto)
6. **NanoChemistry** (Coordinators: Jaume Veciana & David Amabilino)

Scientific Programme - WG

Tuesday March 21, 2006

Scientific Programme - WG		
Tuesday March 21, 2006		
Working Groups (parallel sessions)		
	Molecular Electronics	Pablo Ordejon (ICMAB-CSIC, Spain)
	Nanofabrication	Francesc Perez Murano (CNM, Spain)
	Nanobiotechnology	Laura Lechuga (IMM-CNM-CSIC)
17h30-20h00	Nanoenergy	17h30-17h45 Javier Sanchez (Carburros Metalicos/MATGAS)
		17h45-18h00 Oscar Miguel (CIDETEC)
		18h00-18h15 M.P. Pina (Universidad de Zaragoza)
		18h15-18h30 J.R. Morante (UB/CeRMAE)
		18h30-18h45 Xavier Obradors (ICMAB/CeRMAE)
	Industrial	17h30-17h45 Isabel Obieta (Inasmet) "Nanomaterials: Opportunities and Challenges "
		17h45-18h00 Javier García (Aenor) "Nanotechnologies Standardisation"
		18h00-18h15 Cesar Merino (Grupo Antolin) "Structural and Surface Characterization of Ni-derived Carbon Nanofibers by Floating Catalyst Method"
		18h15-18h30 Eugenio Vilanova (Universidad Miguel Hernandez de Elche) "The usual strategy to evaluate safety of chemicals can be applied to products developed under nanoscience or nanotechnology?."
		18h30-18h45 Emilio Prieto (CEM) "Quantitative nanotechnology – the role of nanometrology"
		18h45-19h00 Carles Escolano (Willems & van den Wildenberg) "Nanomaterials Roadmap"
		19h00-19h15 Rafael Muguerza Eraso (Gobierno de Navarra)
		19h15-20h00 Discussion
	Nanochemistry	17h30-17h45 Jose C. Conesa (ICP-CSIC)
		17h45-18h00 Carmen Ocal (ICMM-CSIC)
		18h00-18h15 Jose Luis Serrano (INA)
		18h15-18h30 Conxita Solans (IIQAB-CSIC)
21h30	Conference Dinner (Restaurant: Palacio Castillo de Gorraiz)	

Pamplona 20-23, March 2006



3rd NANOSPAIN WORKSHOP

WORKING GROUP

Industrial

Speaker: Mr. Carles Escolano
Organisation: Willems & van den Wildenberg España S.L.
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Type of contribution: Presentation
Topic: Nanotechnology in industry

Abstract title: Nanomaterials technology roadmap: horizon 2015

The presentation will introduce the technology roadmaps in the field of nanomaterials that W&W has executed within the NANOROADMAP project completed by December 2005. The horizon for the roadmapping exercise is 2015.

The main objective of a technology roadmap is to gather expert opinions about future technology developments and to build up future scenarios. Because these scenarios are based on the opinion of experts both from industry and research, the resulting roadmap could be considered as a shared view on how technology might develop. Therefore, roadmaps become a useful tool to support the strategic decision-making process on where and how to focus (scarce) R&D resources. For instance, it allows identifying areas where, because of the risk or the level of resources required, are more suitable for collaborative research and/or markets development.

Following a quick scan of 12 different areas within the broad field of nanomaterials (e.g. nanotubes, molecular electronics, quantum dots, etc.), the NANOROADMAP consortium and the EC selected 4: nanoparticles (including nanocomposites), thin films & coatings, dendrimers and nanoporous materials. W&W has executed a technology roadmap for each of these topics.

The presentation will focus both on the approach being followed as well as on the results obtained and how could they be used. W&W will present a short overview of the content of one of these roadmaps including: materials' properties, production processes and major bottlenecks to be addressed and potential market applications. Charts giving an overview of the broad range of potential applications and their status (now, in 2010 and 2015) will be introduced, highlighting differences in potential market growth and risk of failure. Finally, W&W will show how these roadmaps are being put into practice by several research institutes from CSIC to identify business opportunities and, at the end, to reach a greater exploitation of R&D results.

Because the project's results would mostly be public, many organisations could use them to define/align their R&D activities to ensure a greater impact on business and society.

The NANOROADMAP project (www.nanoroadmap.it) was a Strategic Support Action within the 6th RTD Framework Programme and has been funded by the European Commission (EC) to be used as an input to the 7th Framework Programme definition. The consortium gathered 8 organisations from all over Europe to execute 3 technology roadmaps on the field of materials, energy and health and medical systems. Within this consortium, W&W was responsible for leading the nanomaterial roadmap, based in a Delphi-like panel in which a pool of over 100 worldwide experts has participated.

NANOTECHNOLOGIES STANDARDISATION

by Javier GARCIA, Head of Unit ISO/CEN - AENOR

Why is standardization necessary in the field of nanotechnology?

As technology moves out of the human scale it becomes more difficult to measure critical features associated with it and more difficult to be certain that you have control over the processes used. As the critical scales approach the dimensions of atoms the difficulties become compounded. Characterization and analytical techniques become more complex to use, more dependent on control technologies and may not even be available. System calibration may have to be based on different or new principles, and qualification and certification of calibration procedures become much more difficult.

All of these issues, together with others, point to a need for standardization for nanotechnologies. In addition, there is a pressing need for a commonly agreed and accepted terminology to allow the accurate, unambiguous description of nanomaterials and systems.

With these words, Dr. Peter Hatto, Director of Research for Ionbond Ltd, and Chairman of the International Standardisation Committee ISO/TC 229 “Nanotechnologies”, justifies the need to develop standardisation works in the field of nanotechnologies.

The Spanish Association for Standardisation and Certification, , AENOR (www.aenor.es), is an entity dedicated to develop standardisation and certification activities (S+C) in all industrial and services sectors with the aim of contributing to improve the quality and the competitiveness of organizations, as well as to protect the environment.

AENOR, as the Spanish member of both, the European Committee for Standardisation, CEN (www.cenorm.be), and the International Standardisation Organization, ISO (www.iso.org), channels the representation of the interests and knowledge of Spanish experts in all fields through the respective Standardisation Technical Committees.

The increase of nanotechnologies in the recent past, together with the huge perspectives of market growth, make it necessary to improve the understanding and control of matter and processes at the nanoscale, typically, but not exclusively, below 100 nanometres in one or more dimensions where the onset of sizedependent phenomena usually enables novel applications.

Similarly, it is of great importance to determine how to utilize the properties of nanoscale materials that differ from the properties of individual atoms, molecules, and bulk matter, to create improved materials, devices, and systems that exploit these new properties

The standardisation works that are just now beginning include developing standards for: terminology and nomenclature; metrology and instrumentation, including specifications for reference materials; test methodologies; modelling and simulation; and science-based health, safety, and environmental practices.

From AENOR, with the recent creation of the standardisation technical body AEN/GET 15 “Nanotecnologías”, we shall have available the forum to follow the works of the European and International standardisation technical committees CEN/TC 352 & ISO/TC 229.

AEN/GET 15 will contribute to the development of robust standards and other deliverables relevant to nanotechnologies that will:

- Support the sustainable and responsible development and global dissemination of these emerging technologies;
- Facilitate global trade in nanotechnologies, nanotechnology products and nanotechnology enabled systems and products;
- Improve quality, safety, security, consumer and environmental protection, together with the rational use of natural resources in the context of nanotechnologies;
- Promote good practice in the production, use and disposal of nanomaterials, nanotechnology products and nanotechnology enabled systems and products.

Some of the topics that will probably contribute to develop standards necessary to the nanotechnologies field are:

- terminology for nanotechnology(ies);
- protocols for toxicity testing of nanoparticles;
- standardized protocols for evaluating environmental impact of nanoparticles;
- “methods of test” for nanoscale devices and nanostructured materials;
- measurement techniques and instruments;
- calibration procedures and certified references materials, and
- new standards for multifunction nanotechnology systems and devices.

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STRUCTURAL AND SURFACE CHARACTERIZATION OF NICKEL-DERIVED CARBON NANOFIBERS BY FLOATING CATALYST METHOD.

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During past few years a considerable interest has been generated for using carbon nanofibers (CNF) and carbon nanotubes (CNT) as a filler for improving the electrical and mechanical properties of polymer composites. The unique and high values of aspect ratio, strength and modulus of carbon nanofibers are the factors that leads to such conclusions (^{1,2}). It is also well known that a strong fiber-matrix interface is required for adequate mechanical reinforcement in polymer composites with glass or regular carbon fibers. The interaction on the fiber-matrix interface is governed by the surface properties of the fiber as well as those of the matrix and, in particular their surface energies.

CNF production and technology was leaded in either Japan and North America in the last two decades. Recently, Grupo Antolín Ingeniería has become the first and only European producer of Carbon Nanofibers. GANF1 product is first ever reported CNF grown using nickel as a catalyst through the floating catalyst method. Natural gas was used as a carbon feedstock.. The quality of the produced nanofibres is very good, with high aspect ratios (as shown in a SEM picture in figure 1). Among the different reported catalytic carbon nanofiber structure, GANF1 has a highly graphitic stacked cup structure, which consist in a spiral alignment of a graphene layer along an axis, like forming an array of truncated cones with a wide hollow core (as shown in a TEM picture in figure 2). There are some fibrils closed end cones like a bamboo structure. It is remarkable that the nanofibers does not present any impurity of non-catalytic amorphous carbon, attaining a great conductive properties and graphitic index, which are shown in the Table 1, with other physical properties.

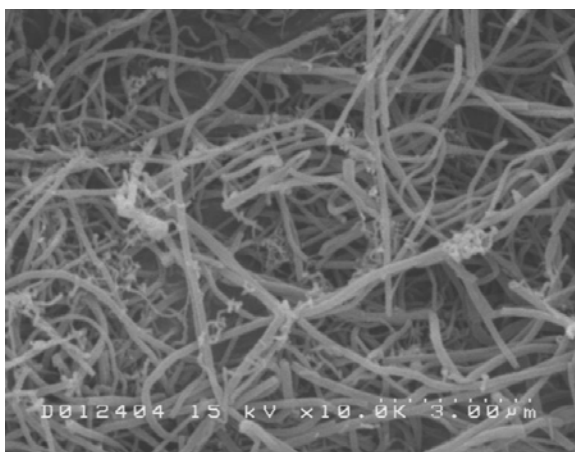


Figure 1. SEM picture of GANF1

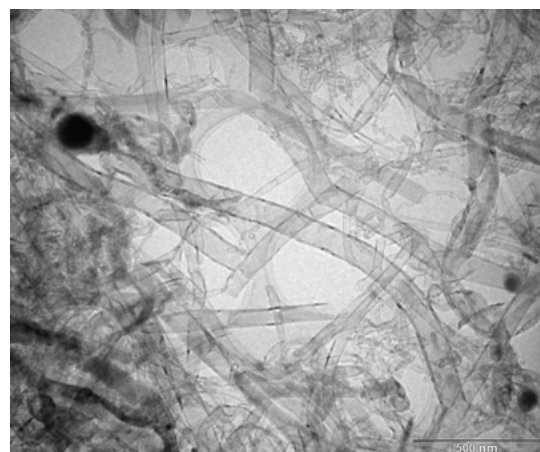


Figure 2. TEM picture of GANF1

Table 1.- GANF1 carbon nanofibres physical properties

PROPERTIES	
Fiber Diameter measured by TEM (nm)	20 – 80
Fiber Length measured by SEM (μm)	> 30
Bulk Density (g.cm^{-3})	> 1.97
Apparent Density of as-Grown Nanofibers (g.cm^{-3})	0.009
Apparent Density of Stripped and Debulked Nanofibers (g.cm^{-3})	0.060
Specific Surface Area –BET ($\text{m}^2.\text{g}^{-1}$)	150 – 200
Graphitization Degree (%)	70
Electrical Resistivity (Ohm.m)	1.10^{-3}
Metallic Particle Content (%)	6 – 8

Surface chemistry characterization was determined for the as grown GANF1, and three surface treated samples: a) pyrolyzed at 500 °C, b) oxydized in air at 350°C, and c) oxydized with H₂O at 700°C. Surface characterization was carried out by means of the Wicking technique. This method permits to measure the contact angle of any liquid which moves into a glass capillary. By using different liquids it is possible to determine the dispersive (γ_s^d), positive (γ_s^+) and negative charge (γ_s^-) surface energy components of any solid surfaces (³⁻⁴). Table 2 gives the surface energy values of as grown and surface treated GANF1 This Table also gives the surface character of these nanofibers as a function of their positive/negative and dispersive/polar ratios.

Table 1.- Surface energies (in mJ.m^{-2}) and surface character of GANF1 carbon nanofibers

GANF1	γ_s^d	γ_s^+	γ_s^-	γ_s^P	γ_s^T	γ_s^+/γ_s^-	γ_s^d/γ_s^P
As-grown	23	0.1	42.1	3.5	26.5	0.002	6.57
Pyrolyzed in N ₂	25	0.6	14.1	6.0	31.0	0.042	4.17
Oxydized with Air	23	1.5	10.7	8.0	31.0	0.140	2.87
Oxydized with H ₂ O	18.6	18.4	12.5	30.3	48.9	1.472	0.61

Data of this Table 2 show that as-grown GANF1 has low surface energy (26.5 mJ.m^{-2}) and that such surface has both high negative charge and high dispersive characters ($\gamma_s^+/\gamma_s^- = 0.002$; $\gamma_s^d/\gamma_s^P = 6.57$). When the GANF1 is pyrolyzed in nitrogen both dispersive becomes more important with respect to polar components. Oxidation in air increases of the positive polar component of the surface of GANF1, keeping the same dispersive values. And finally, the surface treatment in H₂O at 700 °C produces a hugh increase of the polar surface sites, which indicates that water deeply modifies the surface.

In summary, the GANF1 carbon nanofibers produced by the Grupo Antolín Ingeniería present an excellent quality, with a high graphitic structure. In adition, GANF1 has a surface which can be easily modified for different applications.

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NANOMATERIALS: OPPORTUNITIES AND CHALLENGES

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Nanotechnologies are regarded world-wide as key technologies of the 21st Century. Nanotechnological products and processes hold an enormous economic potential for the markets of the future. The production of ever smaller, faster and more efficient products with acceptable price-to-performance ratio has become an increasingly important success factor in the international competition of many sectors. In this context, improvements based on these technologies are to be considered both in a short to medium-term time scale as well as on a long-term basis in view of visionary applications.

Various **applications** feasible in a short to medium-term time horizon like:

- a) lightweight and mechanically outstanding structures based on nano-composites, specially for harsh environments, high temperatures,...
- b) improved and smaller systems and controls based on microsensors, on smart nanomaterials and/or on embedded actuators for on-line monitoring, self-calibration, self-regulation, or self-healing applications
- c) Thermal and mechanical protection layers with outstanding tribological characteristics for engine parts made of nanostructured materials
- d) Filtration, cleaning and absorption of non-wanted specimen obtained from aerogels
- e) And many others related, to anti-stain textiles, anti-corrosion paintings, heat-absorbing or anti-reflection windows, etc.. based on multi-functional nanomaterials

The long-term applications are based on strategic actuations like imitating nature or on molecular nanotechnologies, where material synthesis “a la carte” can be expected and applications in biomedical devices are envisaged.

Anyhow, all these opportunities will be possible if all the challenges that these new technologies imply can be overcome:

- a) Technical challenges: the manipulation and observation of the materials and systems of micro and nanoscopic size is not obvious. These materials tend to agglomerate, are difficult to disperse and can not be well characterized

- b) Regulations and standards: are another important aspect in these new technologies, as many concerns are arising in terms of toxicological impact as well as in the standardization of the specifications
- c) Cost and quantities: can be another issue while these materials are under development as no major manufacturer is willing to produce big quantities, price can not lower to acceptable numbers

Once those challenges are addressed the impact of nanotechnologies will be enormous, especially in technology-demanding sectors.

The presentation will highlight the development of nanotechnologies based on nanoscale design and materials, referring to Inasmet activities in Nanomaterials. Some of the challenges that are being faced will be described.

QUANTITATIVE NANOTECHNOLOGY – THE ROLE OF NANOMETROLOGY

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It is clear that Nanotechnology is since last years a continuous revolution in the world of science, influencing the full Society because the great diversity of practical applications in all fields.

After the last advances in fundamental nanoscience, design of new nanomaterials and ultimately the manufacturing of new nanoscale products, the difficulty in reaching the nanoscale design expectations fulfilling the incredible very narrow specifications depend in high degree on the capability of measuring properties and performance characteristics in an accurate and reproducible way [1].

Such measuring capability should include the traceability [2][3] to the corresponding basic unit of the International System (S.I.), in most of cases, the length unit, the meter, but also to other relevant units as f.i., the unit of force, the newton [4], as the only way to be able to compare realizations and manufactured parts and devices produced by different techniques and in different places in our today's global world.

Nanotechnology depends highly from instrumentation and metrology. The remarkable progress of today's nanotechnology is in some way a result of the evolution suffered by the instrumentation and metrological methods applied to nanoscale measurements.

But currently available metrology tools have partially reached in some specific fields the limits of resolution and accuracy and it is sure that without a new evolution they won't be able to meet future requirements for nanotechnology or nanomanufacturing. New techniques, tools, instruments and infrastructure will be needed to support a successful nanomanufacturing industry [1].

Looking for instance at the International Technology Roadmap for Semiconductors in its 2005 edition [5], most of the forecast on technologies for the future, even at short term, do not have yet the answer to how to produce the different devices, due to the critical dimensions needed at such level of integration.

The difficulty for assuring the fulfillment of very narrow tolerances derives from the uncertainty of the measuring instrument. Although the ideal tolerance/uncertainty ratio should be 10, at the nanoscale it is nearly impossible to get such value, being more frequent to reach values less than 3 and in worst cases 1. So, revolutionary more than evolutionary approaches to nanometrology are required for the very near future.

The natural way to reduce the uncertainty of measuring instruments used in nanometrology is to produce more accurate standards [6] and/or reduce the number of calibration steps from the practical realization of the basic unit. The first approach implies new manufacturing nanotechniques and the second one to convert manufacturing equipment and manipulators in metrological instruments by combining them f.i. with optical and X-ray interferometers and by developing 3D [7][8] and molecular measuring machines [9], many of them built around of or integrating SPM probes with improved tips [10][11] or a better calibrated ones [12].

Many new developments have already been made in some National Institutes of Metrology [2][3][13] resulting in suitable standards and metrological instruments. By means of interlaboratory key comparisons (<http://kcdb.bipm.org>), NMIs obtain information on how good are their results compared to the reference value and to each other. This is the first step to improve the metrological features of instruments and hence SPMs and other manufacturing and manipulating tools used in nanotechnology after incorporating these improvements in the production line.

In our presentation we offer a general overview of this revolutionary on-going process directed to implement an improved nanotechnology for the future with a high degree of confidence in the performance of mass production devices, supported by the crucial role that nanometrology plays in such process.

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THE USUAL STRATEGY TO EVALUATE SAFETY OF CHEMICALS CAN BE APPLIED TO PRODUCTS DEVELOPED UNDER NANOSCIENCE OR NANOTECHNOLOGY?

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The presentation of the reports about Nanoscience and Nanotechnology in Spain, is said something like: Nanoscience (more extended the term "nanotechnology") is the knowledge and methodologies to study, producing and characterising functional structures of dimensions of nanometers; this study include analysis, properties (structural, mechanic, electric, magnetic, chemical) interaction with other nanostructures, with electromagnetic radiations and "**interaction with biological media**". This last "interaction" is the key question to understand the safety of something (product, material, process) that is wanted to be put in the market and can intentionally or accidentally interact with humans (operators or consumers) or with the environment (ecosystem or public human environment).

Pharmaceutical industry has very clear that from the early beginning of the development of a molecule for a potential application a evaluation of the safety should be in parallel with the evaluation of the efficacy and applicability. Most of the thousands of chemicals tested are discarded for further development and investment due to the early conclusion that this molecule will not pass the requirement for safety in the process of registration (notification, evaluation and authorization). This is no so clearly approached in other fields developing new product, considering only the expected desired properties. Safety evaluation is needed from the early beginning in order avoid to direct the technological development through a way without no exit because the product show an intrinsic hazards which will not allow to be put in the market due to risks for human or for the environment. However if a product want to arrive to a final real possibility to be put in the market, safety should be considered from early beginning and to allow to choose among the different options, that which offers appropriate safety (not always the best under efficiency criteria).

The experience in evaluation to chemicals (agrochemicals, biocides, foods additives, cosmetics, human or veterinarian drugs, and industrial chemicals) during last decades have been proved his efficiency (with some uncertainty) in guaranty the safety applications if the appropriate studies are performed for classification of hazards and risk assessment. Risk evaluation needs at least two main groups of data: (1) Data of the toxicity (**effects**) and its quantification for establishing which could be the safety dose that could be accepted without effects (for human or ecosystems) or with acceptable low probability of causing effects. (2) Evaluation and estimation of the **exposure** that is caused to humans and ecosystems by the production, handling, commercialization and use of the products containing the chemical under evaluation. The final step is the **risk characterisation** using both sets of data.

The toxicological evaluation involves studies done under acceptable protocols and quality. Protocols has been developed either to evaluate effects in humans (by in vitro and animal testing) and for evaluating effect to the environment in aquatic, terrestrial and soil ecosystems. A key question is if the usual protocols and criteria for evaluation of chemical can be extrapolated to new products developed from nanotechnology.

For human toxicity the usual first primary studies are related with skin irritation, immune response (skin sensitisation). Dermal penetration uses to be a key factor for evaluation and is

probably a key factor (together with lung absorption) to understanding the risk for application of nanoparticles. The absorption, distribution and bio-availability to target organs and cells, most probably need especial considerations. In fact, the potential peculiar possibilities of nano-structures are the reasons of considering application in nanomedicine for directing drugs to the desired tissue or cells. The pass through living barriers (as placenta, nerve-blood barrier) represents special consideration to evaluate neurotoxicological and reproduction effects.

Evaluation of human exposure (modelling and monitoring) needs to have appropriate detection quantification procedures. The environmental fate and route for exposure to aquatic and terrestrial ecosystem will require some new approaches, as well as strategies for residual management, disposals, elimination and remediation (including biotechnological approaches for bioremediation).

In conclusion, more questions are coming than appropriate responses we have but this does not justify delaying to address the evaluation of safety of new product as part of the early development.

Pamplona 20-23, March 2006



3rd NANOSPAIN WORKSHOP

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Pamplona 20-23, March 2006



3rd NANOSPAIN WORKSHOP

LIST OF PARTICIPANTS

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Dybek	Aneta	University of London	United Kingdom	Poster
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Jiménez Jiménez	David	<i>Universitat Autònoma de Barcelona</i>	Spain	Poster
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Kristensen	Anders	<i>Technical University of Denmark</i>	Denmark	Keynote
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López Arbeloa	Fernando	<i>Universidad del País Vasco</i>	Spain	Poster
López Arraiza	Alberto	<i>Universidad del País Vasco</i>	Spain	Poster
López Cartes	Carlos	<i>ICMSE-CSIC</i>	Spain	Poster
López del Río	Tatiana	<i>Universidad de Santiago de Compostela</i>	Spain	Poster
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López-Tendero	María José	<i>AIDICO-RENAC</i>	Spain	Poster
Lorente	Nicolas	<i>Université Paul Sabatier</i>	France	Keynote
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Muñoz	Edgar	Instituto de Carboquímica - CSIC	Spain	Poster
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Nolla	Jordi	IQAB-CSIC	Spain	Poster
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Pasán	Jorge	Universidad La Laguna	Spain	Poster
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Quirós	Carlos	Universidad de Oviedo	Spain	Poster
Ragusa	Andrea	CSIC	Spain	Poster
Ramón Valencia	Bladimir Azdrubal	Universidad del País Vasco	Spain	Poster
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Sanchez	Florencio	<i>ICMAB-CSIC</i>	Spain	Attendee
Sanchez Portal	Daniel	<i>DIPC</i>	Spain	Oral
Sanchez-Cortes	Santiago	<i>Instituto de Estructura de la Materia</i>	Spain	Poster
Schift	Helmut	<i>Paul Scherrer Institut</i>	Switzerland	Keynote
Serrano	José Luis	<i>Instituto de Nanociencia de Aragón</i>	Spain	Attendee
Silkin	Vyacheslav	<i>Donostia International Physics Center</i>	Spain	Poster
Smit	Roel	<i>Universidad Autonoma de Madrid</i>	Spain	Attendee
Solans	Conxita	<i>IIQAB-CSIC</i>	Spain	Attendee
Soriano	Leonardo	<i>Universidad Autónoma de Madrid</i>	Spain	Poster
Soriano Portillo	Alejandra	<i>ICMOL -Instituto Ciencia Molecular</i>	Spain	Poster
Tamayo	Javier	<i>CSIC/IMM-CNM</i>	Spain	Oral
Tarancon Rubio	Albert	<i>CeRMAE-Generalitat de Catalunya</i>	Spain	Poster
Tatay	Sergio	<i>Universidad de Valencia</i>	Spain	Poster
Tejada	Javier	<i>Universidad de Barcelona</i>	Spain	Oral
Thompson	Carl V.	<i>MIT</i>	Spain	Keynote
Toca-Herrera	José L.	<i>Rovira i Virgili University</i>	Spain	Poster
Torrent-Burgués	Joan	<i>UPC-Chemical Engineering, CBEN-CREBEC</i>	Spain	Poster
Torres	Francesc	<i>Universitat Autònoma de Barcelona</i>	Spain	Poster
Toset	Jordi	<i>Universidad de Barcelona</i>	Spain	Oral
Tros de Ilarduya	Conchita	<i>Universidad de Navarra</i>	Spain	Poster
Urtizberea	Ainhoa	<i>Instituto Ciencia de Materiales de Aragon</i>	Spain	Poster
Varela	Fernando	<i>CEMITEC</i>	Spain	Attendee
Vargas	Fernando	<i>Witec</i>	Germany	Poster
Vazquez	Manuel	<i>MEC,ICMM-CSIC</i>	Spain	Oral
Veciana	Jaume	<i>ICMAB-CSIC</i>	Spain	Oral
Velez	Marisela	<i>Universidad Autonoma de Madrid</i>	Spain	Poster
Verges	Jose Antonio	<i>ICMM-CSIC</i>	Spain	Poster-Flash
Vericat	Carolina	<i>Universitat de Barcelona</i>	Spain	Poster
Vilanova	Eugenio	<i>Universidad Miguel Hernandez de Elche</i>	Spain	Attendee
Villanueva Torrijo	Guillermo	<i>IMB-CNM. CSIC</i>	Spain	Poster

Villarán	Maria Carmen	<i>Fundación LEIA</i>	Spain	Attendee
Viviente Sole	Jose Luis	<i>Nanosciences and Nanotechnology - European Commission</i>	Belgium	Keynote
Wintterlin	Joost	<i>Universitaet Muenchen</i>	Germany	Keynote
Yoldi	Maria	<i>University of Navarra</i>	Spain	Poster-Flash
Zabala Martinez	Irene	<i>Universidad Pública de Navarra</i>	Spain	Attendee
Zabaleta	Virginia	<i>University of Navarra</i>	Spain	Poster
Zabalo Zabalegui	Jesús	<i>SODENA</i>	Spain	Attendee
Zuza Hernández	Ester	<i>Universidad del País Vasco</i>	Spain	Poster

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