AL Académie universitaire Louvain

MATERIALS

2014

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The *Académie universitaire Louvain* (AL) is a university consortium composed of the following three academic institutions: *Université catholique de Louvain* (UCL), *Université de Namur* (UNamur) and *Université Saint-Louis* (Saint-Louis).

In this particular case, the brochure "Materials" has been prepared by the Research Administration Departments of the UCL and UNamur only, with the valuable help of a peer review Committee composed of:

- Pr Christian Bailly, UCL - Science and Technology Sector, Institute of Condensed Matter and Nanosciences (IMCN)
- Pr Davide Bonifazi, UNamur - Department of Chemistry and NAmur Research College (NARC)
- Pr Pierre Dehez, UCL - Humanities Sector, Institute for Multidisciplinary Research in Quantitative Modelling and Analysis (IMMAQ)
- Pr Olivier Deparis, UNamur - NAmur Research Institute for LIfe Sciences (NARILIS)
- Pr Anne des Rieux, UCL - Medical Sector, Louvain Drug Research Institute (LDRI)
- Pr Pascal Jacques, UCL - Science and Technology Sector, Institute of Mechanics, Materials and Civil Engineering (iMMC)
- Dr Christelle Saout, UNamur - NAmur Research Institute for LIfe Sciences (NARILIS)

With the contribution of: Céline Dessaucy (UCL), Mohamed Nawfal Ghazzal (UNamur), Christine Guyot (UCL), Anne-Françoise Martin (UCL), Céline Plumat (UCL)

Cover: Functionalised multiwalled carbon nanotubes for biomedical applications - NAmur Research College (NARC) by Davide Bonifazi

Foreword

Materials: societal and economic trends drive fast scientific and technological evolution

Materials, natural or man-made, are the building blocks of the economy and society. They are everywhere and some have been around for a very long time. But today, man-made materials, including those based on natural building blocks, are undergoing a rapid evolution driven by economic and societal forces, in particular as a result of challenges related to global competition, energy conservation, waste reduction and climate change. The present focus on materials from renewable resources (green chemistry) is clearly an example of such an emerging driver.

The development of materials is also facilitated by remarkable technological and scientific advances. The resulting landscape of available materials is now incredibly diverse and ranges from low-cost bulk resources to engineered structural materials and high-tech devices.

The application range has also expanded dramatically. While traditional domains such as construction industry or transport have kept and even increased their relevance, new fields have emerged and are growing rapidly, *e.g.* materials for electronics, biomedical applications and materials for energy harvesting, to name just a few.

Materials design and engineering, and the associated manufacturing processes, are increasingly streamlined and integrated for productivity reasons. They are also ever more strongly rooted in fundamental knowledge, in particular *Materials Science*, which provides a deep understanding of relevant properties on atomic and molecular scale. The ability to grasp and control the structure and properties of materials at the lowest level even leads to a *fusion of materials science and nano-science* in key domains such as nano-electronics and nano-medicine.

Other major scientific and technological trends should be kept in mind. They include:

- *the emergence of digital simulation* to complement and, at times, replace experimental testing; when adequate models are available thanks to theoretical advances, "digital experiments" may indeed prove to be easier, faster and cheaper than real ones;

- *the need and ability to balance multiple properties in a single material*: modern materials must combine a variety of performances, from structural to functional and aesthetic, from bulk to surface; this in turn often requires the understanding and design of new materials based on multiple components and organised on multiple scales, as demonstrated by the fast growth of composites and hybrid materials;

- *the emergence of surface-dominated materials*: very thin materials have been around for a long time, but their relative importance is growing rapidly which is, of course, related in part to the previous trend. Protective coatings and catalytic surfaces are good examples of this;

- *an increased focus on "soft matter":* while hard and strong materials still dominate the field, there is considerably more emphasis nowadays on soft materials than there used to be, *e.g.* gels or even liquids with very specific properties, in particular (but not exclusively) for biomedical and biomechanical applications;

- *the emergence of green chemistry-based materials* with a strong emphasis on CO_2 management and renewable building blocks; how (and to what extent) this trend will eventually affect the whole industrial landscape is still the subject of heated discussion;

- *the multidisciplinary nature of materials science and technology*: even though this is not new, it now completely dominates the picture and is the result of all the trends described above.

Materials at Académie Louvain: academic creativity partnering with society

Académie universitaire Louvain has a strong and longstanding tradition of research and service to society in the area of materials. The present brochure highlights some of the key elements of the research work being currently conducted under its umbrella. The several research teams are at the forefront of the trends highlighted above, be it on the experimental or theoretical side, on bulk or surface materials, hard or soft systems. Based on internationally recognised fundamental expertise, the academic, scientific and technical staff members are partnering with economic actors, locally and internationally, to help develop creative solutions in a tough economic context. Examples of such collaborations that speak for themselves can be found in the many Walloon *Pôles de compétitivité* projects as well as the European projects in which *Académie universitaire Louvain* teams are involved. In addition to these major projects, bilateral collaborations and service activities are also being developed.

Materials research increasingly requires the pooling of multiple expertise and technical capabilities. This evolution is also captured at *Académie universitaire Louvain* by the emergence of technological platforms (some explicitly defined, others more informal) which bring together people and equipment to create a critical mass. The main examples of this are also highlighted in the brochure.

Christian Bailly
Chairman of the peer review Committee

Content

Reading notes pivot table

The pivot table below categorises the reading notes per applications (“Health & safety - Food industry”, “Transport”, “Energy - Environment - Building construction”, “Manufacturing & processes” and “Electromagnetics, photonics & electronics”) and per materials family (“Carbon”, “Composites, hybrids, architectured materials”, “Metals & alloys”, “Ceramics”, “Polymers”, “Gels, supramolecular materials”, “Surfaces coatings, thin films”, “Computational science”, “Biosourced & bioinspired materials”).

	A. • **Health & safety** • **Food industry**	**B.** **Transport**	**C.** • **Energy** • **Environment** • **Building construction**	**D.** **Manufacturing & processes**	**E.** **Electromagnetics, photonics & electronics**
Carbon	A3, A5, A7*, D1, D6, E3, E7, E9, E10*	C1, E3, E9	C1, D1, D6, D8*, E3, E7, E9, E10*, E11*	A5, D1, D4, D6, D8*, E2, E3, E7	C1, E2, E3, E9, E10*, E11*
Composites, hybrids, architectured materials	A5, A6, A7*, D1, D6, E5, E7, E9, E10*	C1, D6, E9, E10*	C1, C2, C4, D1, D6, E5, E7, E9, E10*, E11*	A5, D1, D5, D6, D8*, E7	C1, D6, E5, E6, E8, E9, E10*, E11*
Metals & alloys	A7*, D1, D6, E5, E7	B1	D1, D3, D6, E5, E7	D1, D3, D4, D5, D6, E7, E10*	E5, E6, E11*
Ceramics	A7*, D6, E5		D2, D6, E5	D2, D4, D5, D6, E10*	E5
Polymers	A1, A2, A4, A6, A7*, D6, E7, E9, E10*	C1, D6, E9, E10*	A4, C1, D6 E7, E9	D5, D7*, D8*, E7, E10*	C1, D6, E9, E10*, E11*
Gels, supramolecular materials	A1, A2, A3, A5, A7*, C3, E7		C3, D6, E6, E7	A5, C3, D8* E7	
Surfaces coatings, thin films	A2, A4, A6, A7*, C3, D1, D6, E5, E6, E7, E9	D6, E9	A4, C1, C2, C3, D1, D6, E4, E5, E6, E7, E9, E10*, E11*	C1, C3, D5, D6, E7, E10*, E11*	C1, D6, E5, E4, E6, E9, E10*, E11*
Computational science	A8*		C4, E4	A8*	C2, E1, E2, E4, E10*, E11*
Biosourced & bioinspired materials	A2, A3, A7*, D6, E6, E7	D6	C2, C4, D6, E4, E7	D8*, E7	E4, E10*, E11*

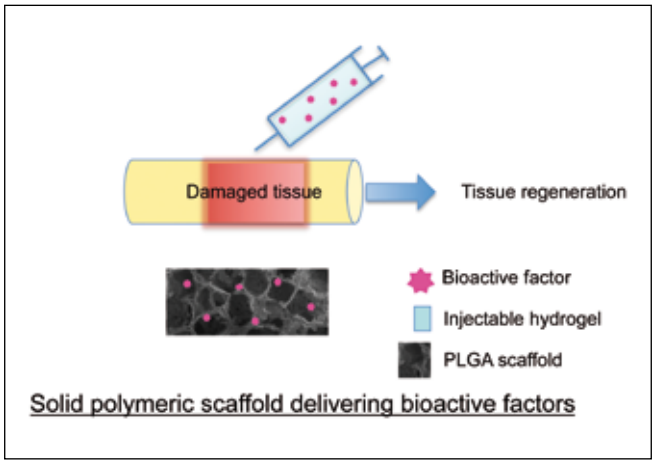
* Technology platform

Biodegradable scaffolds for drug delivery in tissue engineering

SENIOR SCIENTISTS

- Anne DES RIEUX
- Véronique PRÉAT

Research Field and Subjects



The research aims at developing 3D implants (hydrogels, polymeric scaffolds) delivering growth factors, gene therapy, drugs and/or cells that provide sustained delivery factors, support survival, infiltration and proliferation of cells for tissue engineering applications, in particular spinal cord injury.

Mostly, implants are either solid porous scaffolds or injectable hydrogels. While hydrogels could be injectable and thus, provide a better patient compliance (less invasive surgery, good biocompatibility), they often present a low modulus. Scaffolds can be more structured and present stronger mechanical properties, but are less adaptable to the implantation site.

Our core competency lies in the development, characterisation and testing of delivery systems of active factors. One of our interests is to develop implants that would deliver bioactive factors to stimulate tissue regeneration.

Nano- and micro-formulations for the delivery of Vascular Endothelial Growth Factor (VEGF) and Glial Derived Growth Factor (GDNF) were incorporated in either injectable hydrogels or biodegradable polymeric scaffolds. The efficiency of such systems was evaluated *in vitro* as well as *in vivo,* particularly in spinal cord injury models. VEGF nanoparticles loaded in a hydrogel or in a porous poly(lactide-co-glycolide) (PLGA) scaffold stimulated angiogenesis *in vivo*. GDNF delivery from alginate hydrogels supported a functional recovery superior to controls of spinal cord injured rats.

Scaffold-based gene delivery systems such as porous PLGA implants or fibrin-based hydrogels capable of localised transgene expression provide a platform for inductive and cell transplantation approaches in regenerative medicine.

Scaffold-based systems such as porous PLGA implants or injectable hydrogels loaded with bioactive clues delivery systems and/or cells provide a platform for inductive and cell transplantation approaches in regenerative medicine.

Representative References

- ANSORENA E., DE BERDT P., UCAKAR B., SIMÓN-YARZA T., JACOBS D., SCHAKMAN O., JANKOVSKI A., BLANCO-PRIETO M. J., PRÉAT V., DES RIEUX A. Injectable alginate hydrogel loaded with GDNF promotes functional recovery in a rat hemisection model of spinal cord injury. International Journal of Pharmaceutics 455(1-2): 148-158. **2013**.
- DES RIEUX A., DE BERDT P., ANSORENA E., UCAKAR B., JACOBS D., SCHAKMAN O., AUDOUARD E., BOUZIN C., AUHL D., SIMÓN- YARZA T., FERON O., BLANCO-PRIETO M. J., CARMELIET P., BAILLY C., CLOTMAN F., PRÉAT V. Vascular endothelial growth factor-loaded injectable hydrogel enhances plasticity in the injured spinal cord. Journal of Biomedical Materials Research. Part A. *In press.* **2013**.
- DES RIEUX A., UCAKAR B., KAISHUSHA MUPENDWA BILLY PAUL, COLAU D., FERON O., CARMELIET P., PRÉAT V. 3D systems delivering VEGF to promote angiogenesis for tissue engineering. Journal of Controlled Release 150(3): 272-278. **2011**.
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- DES RIEUX A., SHIKANOV A., SHEA L. Fibrin hydrogels for non-viral vector delivery *in vitro*. Journal of Controlled Release 136(2): 148-154. **2009**.

Funding

- Fonds de la Recherche Scientifique (F.R.S.-FNRS)
- Brussels Institute for Research and Innovation (INNOVIRIS), Brains (Back) to Brussels

Partnership

- Northwestern University, Pr L. Shea (USA)
- University of Navarra, Pr M.-J. Blanco-Prieto (Spain)
- Katholieke Universiteit Leuven (KULeuven), VIB Vesalius Research Center (VRC), Pr P. Carmeliet (Belgium)

Main Equipment

- Nanosizer
- Cell culture laboratory
- Small animal surgery equipement
- Tissue sample processing and staining

Keywords

Drug delivery
Nanosystems
Hydrogels
Biodegradable scaffolds
Tissue engineering

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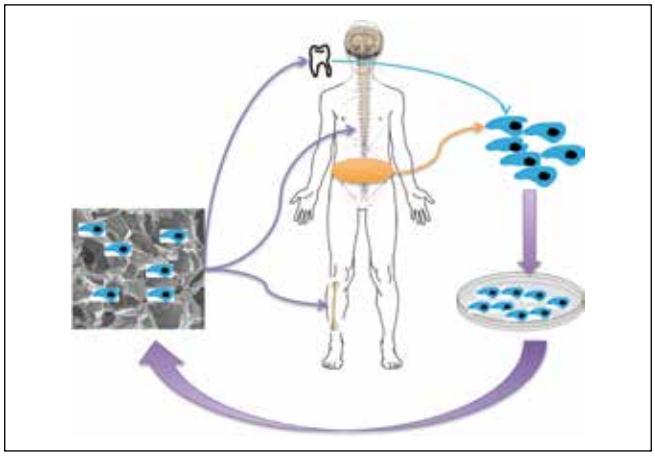
Biomaterials for cellular delivery and tissue engineering

SENIOR SCIENTISTS

- Anne DES RIEUX
- Denis DUFRANE
- Gaëtane LELOUP

Research Field and Subjects



Conventional therapies, including surgical treatments, are not yet sufficient to promote adequate recovery of damaged/failed organs. Strategies to induce and support organ regeneration have attracted great interest. They are mainly based on tissue engineering and consist of the combination of a matrix, stem cells and potential growth factors.

Our core competency lies in the development of biodegradable and biocompatible scaffolds, loaded with stem cells, aiming at tissue regeneration.

Dental stem cells are incorporated in injectable hydrogels, either to stimulate spinal cord or dental regeneration.

Adipose stem cells are grown with demineralised bone matrix and differentiated into osteoblasts *in vitro* to form a 3D structure that can be implanted in large bone defects.

Our scientific approach is multidisciplinary and involves the development of new scaffolds, their characterisation, the evaluation of cell viability and behaviour when incorporated in the scaffold *in vitro* and *in vivo* and the study of their interactions with biological systems.

Representative References

- DES RIEUX A., DE BERDT P., ANSORENA E., UCAKAR B., DAMIEN J., SCHAKMAN O., AUDOUARD E., BOUZIN C., AUHL D., SIMÓN-YARZA T., FERON O., BLANCO-PRIETO M.-J., CARMELIET P., BAILLY C., CLOTMAN F., PRÉAT V. Vascular endothelial growth factor-loaded injectable hydrogel enhances plasticity in the injured spinal cord. Journal of Biomedical Materials Research. Part A. *In press*. **2013**.
- ANSORENA E., DE BERDT P., UCAKAR B., SIMÓN-YARZA T., JACOBS D., SCHAKMAN O., JANKOVSKI O., DEUMENS R., BLANCO-PRIETO M.-J., PRÉAT V., DES RIEUX A. Injectable alginate hydrogel loaded with GDNF promotes functional recovery in a hemisection model of spinal cord injury. International Journal of Pharmaceutics 455(1-2): 148-158. **2013**.
- SCHUBERT T., LAFONT S., BEAURIN G., GRISAY G., BEHETS C., GIANELLO P., DUFRANE D. Critical size bone defect reconstruction by an autologous 3D osteogenic-like tissue derived from differentiated adipose MSCs. Biomaterials 34(18): 4428-4438. **2013**.
- VERITER S., GIANELLO P., IGARASHI Y., BEAURIN G., GHYSELINCK A., AOUASSAR N., JORDAN B., GALLEZ B., DUFRANE D. Improvement of subcutaneous bioartificial pancreas vascularization and function by co-encapsulation of pig islets and mesenchymal stem cells in primates. Cell Transplantation. *In press*. **2013**.
- LEPRINCE J.-G., ZEITLIN B.D., TOLAR M., PETERS O.A. Interactions between immune system and mesenchymal stem cells in dental pulp and periapical tissues. International Endodontic Journal 45(8): 689-701. **2012**.
- SCHUBERT T., XHEMA D., VERITER S., SCHUBERT M., DELLOYE C., GIANELLO P., DUFRANE D. The enhanced performance of bone allografts using osteogenic-differentiated adipose-derived mesenchymal stem cells. Biomaterials 32(34): 8880-8891. **2011**.

Patent

- Multi-dimensional biomaterial and method for producing the same. WO 2010/139792 (A2), 2010. (Application number WO 2010/EP57847, 2010; Priority number EP 2009/0161976, 2009).

Awards

- Paul Van de Velde Prize 2009, Université catholique de Louvain (D. Dufrane)
- Fonds de Biotechnologie - Biotechnologie Fonds: Belgian Biotechnology Fund Awards 2011 for the Best Research on Advanced Therapies (D. Dufrasne)

Funding

- Fonds de la Recherche Scientifique (F.R.S.-FNRS)
- Fédération Wallonie-Bruxelles: Action de Recherche Concertée (ARC)
- Fondation Salus Sanguinis
- Fondation Saint-Luc

Partnership

- University of Texas Health Science Center, San Antonio, Pr A.R. Diogenes (USA)

Main Equipment

- Cell culture laboratory
- Small animal surgery equipment
- Tissue sample processing and staining
- Clean room facility for advanced therapy medicinal product

Products and Services

- Cell isolation, culture and characterisation (stem cells, primary cells)
- Scaffold development
- Preclinical studies in different animal models

Keywords

Adipose stem cells
Dental stem cells
Injectable hydrogels
Regenerative medicine
Cellular therapy

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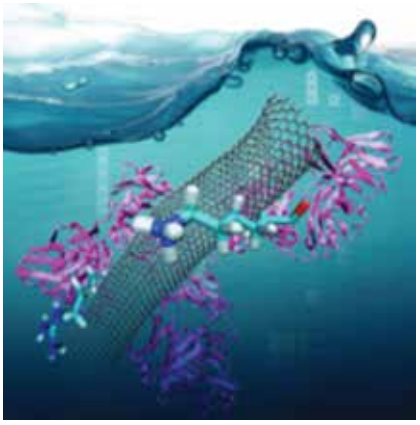
Preparation of carbon-based materials for biochemical studies

SENIOR SCIENTISTS

- Davide BONIFAZI
- Stéphane VINCENT

Research Field and Subjects



Our research unit "*Unité de Chimie Organique*" is focused on the engineering and organic synthesis of molecules, thus aiming at the creation of functional architectures in highly interdisciplinary projects, including material sciences and chemical biology. Synthesis and functionalisation of carbon-based nanostructures are at the heart of the program in carbon-based advanced materials. In particular, a "multidimensional approach" is used in the research, which includes studies of biological substrates with the aim of:

- Developing novel synthetic methodologies for covalent chemistry of highly emitting fluorophores;
- Providing advanced organic materials with exceptional optoelectronic and architectural properties;
- New hybrids for chemical biology applications.

For instance, we recently developed the synthesis of glycosylated fullerenes and pillararenes as a novel class of antibacterial agents. We were able to demonstrate that properly derivatised C60 structures can selectively bind uropathogenic bacteria and prevent their adhesion to their host mammalian cells. Chemistry of this kind can be extended to many other biochemical applications. Focusing on the carbon nanotubes-driven (CNTs-driven) activities, by means of jointly collaborative work, H-bond–driven reversible exohedral solubilisation/functionalisation of multi-walled CNTs (MWCNTs) in apolar organic solvents has been accomplished by a dynamic combination of self-assembly and self–organisation processes. This leads to the formation of supramolecular polymers, which enfold around the outer wall of the MWCNTs and allows for their solubilisation in organic and aqueous solvents. These approaches have been expanded with magnetically-active CNTs. Specifically, Fe-filled MWCNTs (Fe@MWCNTs) were synthesised and functionalised with cancer cells targeting antibody Cetuximab. The resulting "nanomagnets" were able to bind and sort cancer cells in a mixed population with healthy cells, allowing also magnetically-induced selective hyperthermia-mediated killing of the malignant cells.

Representative References

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- MAREGA R., DE LEO F., PINEUX F., SGRINANI J., MAGISTRATO A., NAIK A.D., GARCIA Y., FLAMANT L., MICHIELS C., BONIFAZI D. Functionalized Fe-filled multiwalled carbon nanotubes as multifunctional scaffolds for magnetization of cancer cells. Advanced Functional Materials 23(25): 3173-3184. **2013**.
- MAGGINI L., LIU M., ISHIDA Y., BONIFAZI D. Anisotropically luminescent hydrogels containing magnetically-aligned MWCNTs-Eu(III) hybrids. Advanced Materials 25(17): 2462–2467. **2013**.
- DE LEO F., SGRINANI J., BONIFAZI D., MAGISTRATO A. Structural and dynamic properties of monoclonal antibodies immobilized on CNTs: a computational study. Chemistry 19(37):12281-12293. **2013**.
- DURKA M., BUFFET K., IEHL J., HOLLER M., NIERENGARTEN J.-F., VINCENT S.P. The inhibition of liposaccharide heptosyltransferase Waac with multivalent glycosylated fullerenes: a new mode of glycosyltransferase inhibition. Chemistry 18(2): 641-651. **2012**.
- DURKA M., BUFFET K., IEHL J., HOLLER M., TAGANNA J., NIERENGARTEN J.-F., BOUCKAERT J., VINCENT S.P. The functional valency of dodecamannosylated fullerenes with *Escherichia coli* FimH – Towards novel bacterial antiadhesives. Chemical Communications 47(4): 1321-1323. **2011**.

Patent

- New heptose derivatives and biological applications thereof. WO 2012/073214 (A2), 2012 (Application number WO 2001/IB55404, 2011; Priority number US 20100418491P, 2010).

Awards

- Young Investigator Lectureship 2012, the ISCHIA School of Organic Chemistry (D. Bonifazi)
- ERC Starting Grant 2011, the European Research Council within the 7th Framework Programme (D. Bonifazi)
- G. Ciamician Medal 2010, the Italian Chemical Society (D. Bonifazi)

Funding

- Fonds de la Recherche Scientifique (F.R.S.-FNRS)
- European Union (EU): Marie Curie Initial Training Network (ITN)
- European Research Council (ERC)
- European Commission: 7th Framework Programme
- Service Public de Wallonie (SPW)
- Belgian Science Policy Office (BELSPO): Interuniversity Attraction Poles (IAP)

Partnership

- Collaborations in the frame of numerous projects funded at the national and international level:
- *Academic (non-exhautive list)*: Centre National de la Recherche Scientifique (CNRS) (France), Université de Strasbourg (France), Royal Institute of Technology (Sweden), Consejo Superior de Investigaciones Científicas (CSIC) (Spain), Semmelweis University (Hungary), International Centre of Biodynamics (Romania), Katholiek Universiteit Leuven (KULeuven) (Belgium), Universidade Nova de Lisboa (FFCT-UNL) (Portugal), Consorzio Interuniversitario Nazionale Per La Scienza E Tecnologia Dei Materiali (INSTM) (Italy)
- *Industrial (non-exhaustive list)*: Attana AB, GVS S.p.A, Solvay, Philips, Ynvisible, n-Tec

Main Equipment

- NMR spectrometers
- Mass spectrometers (HPLC-MS and GC-MS)
- HPLC and MPLC
- Full equipment for organic synthesis including a peptide synthesiser
- Elemental analysis and ICP-OEP

Products and Services

- Organic synthesis

Keywords

Fullerenes
Carbon nanotubes
Antibacterial agents
Biochemical tools

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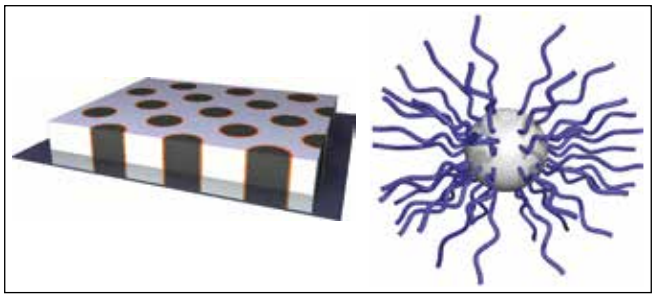
Synthesis and self-assembly in thin films and solutions of stimuli-responsive block copolymers

SENIOR SCIENTISTS

- Charles-André FUSTIN
- Jean-François GOHY

Research Field and Subjects



Responsive polymers attract an ever increasing interest due to their ability to change their properties in response to a small change in their environment. Polymers may be devised to respond to many different stimuli such as pH, temperature, light, redox, ionic strength, etc. In addition, block copolymers can self-assemble in solution or in the bulk to form well-defined nanostructures.

This research topic deals with the development of stimuli-responsive block copolymers for various applications. Different aspects are covered by the research, from synthesis to self-assembly and characterisation. The team has expertise in the synthesis of block copolymers using controlled radical polymerisation methods (RAFT, ATRP, NMP) as well as in the post-functionalisation of polymers. The self-assembly of these block polymers is studied both in solution (formation of micelles) and in thin films.

As examples of realisations, block copolymers bearing a cleavable junction between the two blocks have been synthesised and used as precursors for the preparation of functionalised nanoporous thin films. A photocleavable moiety, a metal-ligand complex, and an ionic bond have been used as junctions. In other examples, light has been used to induce the micellisation of block copolymers or the disruption of preformed micelles, accompanied by the encapsulation or release of a cargo, respectively.

Representative References

- ZHAO H., GU W., THIELKE M.W., STERNER E., TSAI T., RUSSELL T.P., COUGHLIN E.B., THEATO P. Functionalized nanoporous thin films and fibers from photocleavable block copolymers featuring activated esters. Macromolecules 46(13): 5195–5201. **2013**.
- BERTRAND O., FUSTIN C.-A., GOHY J.-F. Multiresponsive micellar systems from photocleavable block copolymers. ACS Macro Letters 1(8): 949-953. **2012**.
- PIOGÉ S., FUSTIN C.-A., GOHY J.-F. Temperature-responsive aqueous micelles from terpyridine end-capped poly(N-isopropylacrylamide)-block-polystyrene diblock copolymers. Macromolecular Rapid Communications 33(6-7): 534-539. **2012**.
- MUGEMANA C., GOHY J.-F., FUSTIN C.-A., Functionalized nanoporous thin films from metallo-supramolecular block copolymers. Langmuir: the ACS Journal of Surfaces and Colloids 28(5): 3018-3023. **2012**.
- BERTRAND O., SCHUMERS J.-M., KUPPAN C., MARCHAND-BRYNAERT J., FUSTIN C.-A., GOHY J.-F. Photo-induced micellization of block copolymers bearing 4,5-dimethoxy-2-nitrobenzyl side groups. Soft Matter 7: 6891-6896. **2011**.

Funding

- Belgian Science Policy Office (BELSPO): Interuniversity Attraction Poles (IAP) VII networks
- European Science Foundation: Precision Polymer Materials (P2M) Network

Partnership

- Université de Liège (ULg), Centre d'Etude et de Recherche sur les Macromolécules (CERM) (Belgium)

Main Equipment

- GPC system (PSS) with triple detection (DRI, UV diode array, MALS)
- Atomic Force Microscope (Nanoscope V, Digital Instrument)
- Dynamic and static light scattering (Malvern-ALV CGS-3 and Vasco system Cordouan Technologies)
- Transmission electron microscopy (LEO922)

Products and Services

- Synthesis of (functionalised) block copolymers by controlled radical polymerisation methods
- Self-assembly and characterisation of block copolymers in thin films (30-300 nm thick)
- Characterisation of colloids and nanoparticles

Keywords

Nanomaterials
Polymer synthesis
Self-assembly
Stimuli responsive materials
Micelles
Vesicles

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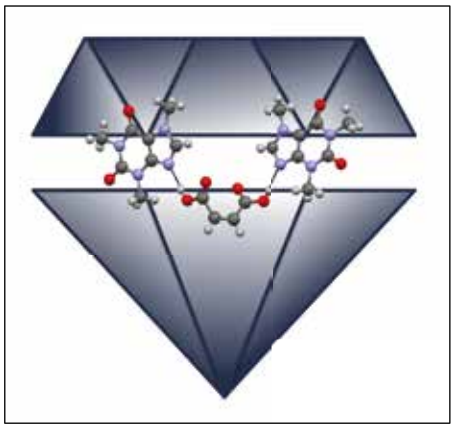
Identification, characterisation, and control of solid state forms of organic compounds: polymorphism, salts, solvates, cocrystals

SENIOR SCIENTISTS

- Tom LEYSSENS
- Johan WOUTERS

Research Field and Subjects



Most organic compounds encountered in the pharmaceutical, chemical and food industries are solid crystalline materials under ambient conditions. Over 90% of all compounds exist in multiple solid forms (polymorphs, hydrates, salts, cocrystals, etc.). Identifying and characterising these solid forms is of crucial importance, not only from a legal point of view (patentability), but also from a practical point of view (process control). The groups of Pr T. Leyssens and Pr J. Wouters are specialised in the identification and characterisation of different solid forms of organic compounds and the use of this knowledge to control the solid form during crystallisation, or to develop novel applications (purification, chiral resolution, etc.). A first research theme, currently under investigation, focuses on the understanding of why and how different crystal forms appear, using a structural experimental and theoretical approach. A second theme deals with understanding the kinetic and thermodynamic aspects of the crystallisation process involving multi-component systems. A third research theme looks into the potential industrial applications of multi-component solid forms, with emphasis on chiral resolution, deracemisation, chemical reactivity in the solid state, purification. Most work is carried out either on pharmaceutically active compounds, or food additives. Types of investigations conducted by our team include:

- Solid state form screening, combined with identification and characterisation of different forms that are identified (polymorphism, salts, cocrystals, etc.) using the equipment mentioned below;
- Development of a robust and up-scalable crystallisation process;
- Development of chiral resolution/purification processes through crystallisation;
- Intervention as external experts in crystallisation/solid state related issues.

Representative References

- TILBORG A., SPRINGUEL G., NORBERG B., WOUTERS J., LEYSSENS T. On the influence of using a zwitterionic coformer for cocrystallization: structural focus on naproxen-proline cocrystals. Crystal Engineering Communications 15(17): 3341-3350. **2013**.
- BRAGA D., GREPIONI F., MAINI L., CAPUCCI D., NANNA S., WOUTERS J., AERTS L., QUERE L. Combining piracetam and lithium salts: ionic cocrystals and co-drugs. Chemical Communications 48(66): 8219-8221. **2012**.
- SPRINGUEL G., LEYSSENS T. Innovative chiral resolution using enantio-specific cocrystallization in solution. Crystal Growth and Design 12(7): 3374-3378. **2012**.
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- TILBORG A., JACQUEMIN D., NORBERG B., PERPETE E., MICHAUX C., WOUTERS J. Structural study of piracetam polymorphs and cocrystals: crystallography redetermination and quantum mechanics calculations. Acta Crystallographica B 67(6): 499-507. **2011**.

Award

- Triannual award of the Royal Society of Chemistry 2008 (Belgium)

Funding

- Fonds de la Recherche Scientifique (F.R.S.-FNRS)
- Fédération Wallonie-Bruxelles: Fonds Spécial de Recherche (FSR) UCL

Partnership

- UCB Pharma S.A.
- Massachusetts Institute of Technology (MIT), Department of Chemical Engineering (USA)
- Centre National de la Recherche Scientifique (CNRS), Centre Interdisciplinaire de Nanoscience de Marseille (CINaM) (France)
- Université catholique de Louvain (UCL) (Belgium)
- Université de Namur (UNamur) (Belgium)
- Università di Bologna, Department of Chemistry (Italy)

Main Equipment

- Basic solid state characterisation (XRPD, FTIR, Raman, Optical Microscopy,…)
- Thermal Analysis (DSC, TGA, HSM,…)
- Chemical Analysis (NMR, HPLC,…)
- *In situ* solution microscopy
- Single Crystal Analysis (XR)
- Crystallisation equipment

Products and Services

- Solid form screening (polymorphism, salts, cocrystals,…)
- Analysis of solid forms
- Thermodynamic analysis of identified forms (phase diagrams, stability,…)
- Single Crystal Analysis (SCA)
- Development and optimisation of crystallisation processes (solid state control, purification, chiral resolution,…)

Keywords

Active pharmaceutical compounds
Food products
Solid state chemistry
Solid forms (polymorphism, salts,…)
Structural characterisation
Thermodynamic analysis
Crystallisation applications

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Functional hybrid nanomaterials and surfaces

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- Karine GLINEL
- Alain JONAS
- Bernard NYSTEN
- Luc PIRAUX

Research Field and Subjects

The research group Functional Hybrid Nanostructures (FHYN) is one of the research groups of the Institute of Condensed Matter and Nanosciences (IMCN). It consists of approximately 35 researchers whose activities are focused on the development and characterisation of functional hybrid nanostructures and smart surfaces in the general areas of spintronics and nanomagnetism, organic electronics (organic thin film transistors, organic non-volatile memories, etc.), multiferroics, bio-medical applications (nano-biosensors, drug delivery, tissue engineering, antibacterial surfaces etc.), corrosion protection, self-cleaning surfaces, nano-actuators, etc.

To achieve these objectives, the members of the group have developed expertises in the following fields:

- Synthesis/fabrication of functional nanostructures: organic, inorganic or hybrid nanowire/nanotube/core-shell arrays, track-etched membranes, alumina templates, etc.;
- Surface modification/functionalisation: nano-/micro-patterning, biofunctionalisation, layer-by-layer assembly, polymer and inorganic nanobrushes synthesis, elaboration of stimuli-responsive layers, etc.;
- Nanoscale characterisation of the structural, physical, and chemical properties of nanomaterials and surfaces using electron and scanning probe microscopy;
- Investigation of the electrical, magnetic, thermal and microwave properties of nanostructured materials.

Representative References

- LECOUVET B., HORION J., D'HAESE C., BAILLY C., NYSTEN B. Elastic modulus of halloysite nanotubes. Nanotechnology 24(10): 105704. **2013**.
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- ANTOHE V.A., GENCE L., SRIVASTAVA S.K., PIRAUX L. Template-free electrodeposition of highly-oriented and aspect-ratio controlled ZnO hexagonal columnar arrays. Nanotechnology 23(29): 255602. **2012**.
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- HU Z., JONAS A.M. Control of crystal orientation in soft nanostructures by nanoimprint lithography. Soft Matter 6: 21-28. **2010**.

Patents

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- Ferroelectric organic memories with ultra-low voltage operation. WO 2009/144310 (A1), 2009 (Application number WO 2009/EP56656, 2009; Priority number GB 2008/0009840, 2008).
- Drug-eluting nanowire array. WO 2009/050168 (A1), 2009 (Application number WO 2008/EP063803, 2008; Priority number EP 2007/0118428, 2007).
- Method and device for high sensitivity and quantitative detection of chemical/biological molecules. WO 2009/010584 (A1), 2009 (Application number WO 2008/EP59460, 2008; Priority number EP 2007/0014037, 2007).

Funding

- European Commission: 7th Framework Programme, Marie Curie Actions
- European Consortium for Accreditation
- Fonds de la Recherche Scientifique (F.R.S.-FNRS)
- Fonds de la Recherche Scientifique (F.R.S.-FNRS): Fonds pour la Formation à la Recherche dans l'Industrie et l'Agriculture (FRIA)
- Belgian Science Policy Office (BELSPO): Interuniversity Attraction Poles (IAP) VII networks
- Fédération Wallonie-Bruxelles: Action de Recherche concertée (ARC)
- Service Public de Wallonie (SPW)
- Fondation Louvain

Partnership

- Most Belgian Universities (within the frame of IAP networks and Wallonia funded projects) and Research Centres (Materia Nova, Certech, etc.)
- Foreign Universities: Groeningen (the Netherlands), Cambridge (United Kingdom), Bordeaux (France), Nancy I (France), Paris 6 (France), Grenoble INPG & UJF (France), CNRS/THALES (France), CEA-Grenoble (France), Institut Pasteur (France), Lausanne EPFL (Switzerland), Nebraska (USA), Nevada (USA), Soochow (China), Rio de Janeiro (Brasil), San Luis Potosi (Mexico), etc.
- Companies: Solvay Solexis, STMicro-electronics, IMEC, Holst, it4ip, EADS, Neurotech, Zentech, THALES Alenia Space S.A, THALES Systèmes Aéroportés S.A., L'ORÉAL, CYTOO, AGC Flat Glass Europe, etc.

Main Equipment

- Hybrid nanostructures fabrication: electrochemical synthesis facilities, high vacuum coating systems (sputtering and e-beam), platform for surface functionalisation, electron beam nanolithography, nanoimprint lithography, photolithography, etc.
- Microscopies:
  - Transmission and Scanning Electron Microscopies (TEM, SEM)
  - Scanning Probe Microcopies (STM, C-AFM, LFM, FMM, Tapping™ mode, Harmonix™ mode, MFM, EFM, KPFM, PFM)
  - Fluorescence microscopy
- Thin film characterisation: X-ray reflectometry, spectroscopic ellipsometry, contact angle measurement
- Set-up for electrical and thermal measurements, SQUID and AGM magnetometers, cryogenics systems, network analysers, etc.

Products and Services

- Fabrication and characterisation tools for hybrid nanostructures (thin films, nanowires, nanotubes, nano-patterned surfaces, etc.)
- Thin metal film deposition vacuum coating

Keywords

Bio-functionalisation
Biosensors
Hybrid functionals
Nanomagnetism & ferroelectricity
Organic electronics
Smart coatings
Spintronics
Templating

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Technology platform: The Namur Nanosafety Centre (NNC) A multidisciplinary platform for the toxicity assessment of nanomaterials

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- Christelle SAOUT
- Stéphane LUCAS
- Jean-Michel Dogné

Research Field and Subjects

namur nanosafety centre
INTEGRATED PLATFORM

In coming years, products based on nanotechnology are expected to impact nearly all industries and will enter consumer markets in large quantities. However, the unique physicochemical properties of manufactured nanomaterials (NM) that make them attractive for manufacturers, also give rise to concerns about their potential adverse effects on human health and the environment. Indeed, due to their nanoscale dimensions, nanoparticles can be easily taken up by cells and exhibit a high surface area per unit mass, leading to an increased potential for biological interactions and activity.

In order to fill a critical knowledge gap, *i.e.* a better understanding of the mechanisms that trigger NM toxicity, the *Université de Namur* has set up a multidisciplinary platform that includes physicists, biologists, and pharmacists who are working together to develop relevant toxicity assays for NM safety assessment. Particular attention is given to compliance with the OECD Guidelines for the Testing of Chemicals, with the EU policies on cosmetics (*Council Directive 2003/15/EC*) and chemicals (REACH). Since NM toxicity is clearly influenced by nanoparticle-specific properties, an extensive characterisation of nanoparticle properties and validation of test systems are performed.

The Namur Nanosafety Centre (NNC) has gained outstanding expertise in nanosafety through its participation in various high-level research programmes leading to the developmentof adapted methods for:

- NM physicochemical characterisation (pristine forms, dispersions and complex matrices including food);
- NM fate and biodistribution studies;
- NM toxicity assessment (*in vitro* and *in vivo* testing);
- Animal whole-body exposure to well-characterised airborne nanoaerosols;
- Hemocompatibility;
- NP-induced changes in cellular signalling and gene expression at transcriptomic and proteomic levels.

The NNC also participates in the metrology, cross-validation and standardisation of assays for regulatory purposes.

Representative References

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Patents

- Radiotherapy device and method. WO 2006/063419 (A1), 2006 (Application number WO 2005/BE00187, 2005; Priority number US 2004/0637480P, 2004).
- Radioactive device. WO 2006/063418 (A2), 2006 (Application number WO 2005/BE00185, 2005; Priority number EP 2004/0447284, 2004).
- Nanocomposites: products, process for obtaining them and uses thereof. WO 03078315 (A2), 2003 (Application number WO 2003/BE00049, 2003; Priority numbers EP 2002/0447039, 2002 – EP 2002/0447166, 2002).

Funding

- Université de Namur (UNamur)
- Service Public de Wallonie (SPW), Direction Générale Opérationnelle de l'Economie, de l'Emploi et de la Recherche (DGO6)
- Service Public de Wallonie (SPW), Plan Marshall
- European Commission: 7th Framework Programme

Partnership

- European Commission, Joint Research Centre (JRC), Institute for Reference Materials and Measurements (IRMM) (Belgium)

Main Equipment

- For NM physicochemical characterisation:
  - 2 MeV Tandetron linear accelerator (Altaïs) for nuclear reactions based spectroscopy;
  - Field Emission Gun - Scanning Electron Microscope JSM-7500F /Jeol (resolution 0.6 nm) with EDX detector[a];
  - CPS 24000 Disc Centrifuge for nanoparticle size analysis[a].

  [a] Equipment validated by the IRMM-JRC (EC) for nanoparticle characterisation studies
- For NM toxicity assessment:
  - *In vivo / ex vivo* testing:
    - Impact-R®, PFA-100®, light transmission aggregometry, electron microscopy, KC-10®, cTGT for NM impact on blood
    - Whole body inhalation exposure models for rodents equipped with RBG-1000® (aerosol generator) and ELPI® (aerosol analyzer)
  - *In vitro* testing:
    - Cell culture platforms for *in vitro* studies (cytotoxicity, proliferation, differentiation, oxidative stress, pro-inflammatory response) using a variety of mouse and human cell lines and primary cells
    - Confocal microscopy (Leica TCS SP5)
    - Gene expression profiling platform: NanoDrop™ spectrophotometer, Agilent Bioanalizer, 7900HT Fast Real-Time PCR system
    - Proteomic platform: 2D-DIGE technology; Typhoon Confocal scanner and DeCyder 2D Software; 1- an ion trap HCT ultra (Bruker) with the possibility of electron-transfer dissociation (ETD) fragmentation; Dionex Ultimate 3000 nanoLC system; 2- a maXis (Bruker) mass spectrometer; 2D-LC system for gel free analysis

Products and Services

- Physico-chemical characterisation (size, distribution and morphology)
- Multielemental determination in complex matrices (solid and liquid)
- Human health impact assessment (*in vivo*, *ex vivo* and *in vitro* testing): cutaneous, digestive, respiratory and blood exposure studies

Keywords

Nanomaterials
Human health
Physico-chemical characterisation
Toxicity assessment
Hemocompatibility
Whole-body exposure
In vivo and *in vitro* assays
Regulatory testing

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http://www.unamur.be/sciences/biologie/urbc
http://www.unamur.be/sciences/physique/larn
http://www.unamur.be/medecine/pharmacie

Technology platform: Statistical Methodology and Computing Support (SMCS)
Statistical services, from numbers to models to understanding

SENIOR SCIENTISTS

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- Alain GUILLET
- Nathalie LEFEVRE
- Catherine LEGRAND
- Arnaud POLLARIS
- Catherine RASSE
- Christian RITTER
- Matthieu VAN PACHTERBEKE

Research Field and Subjects

Efficient extraction of information is essential in materials sciences and this calls for professional statistical analysis. In this context, a technology platform called Statistical Methodology and Computing Support (SMCS) provides assistance in statistical analysis to all researchers at UCL. The SMCS offers consultancy, training, and collaborations.

SMCS performances by domain:

- Quality control: assistance in tests to gain understanding of the sources of measurement errors; design and implementation of systematic methods to monitor measurement processes. For example: determination of measurement system accuracy in the resistance test of a concrete core sample.
- Statistical design of experiments: efficient arrangements of trials to obtain information taking into account measurement and experimentation variability. For example: setting up a design that enables building features to be taken into account in the assessment of a solar screen.
- Analysis and modelling of large data sets common to materials science: often large collections of spectra and other measurements are used to characterise materials. The SMCS can help to extract the relevant information from these large data sets.
- Reliability studies: design and analysis of experiments to determine the durability of materials and their properties. For example: analysis of intralaboratory traction test of 12.5 mm prestressing steel strand.

Representative References

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- BUGLI C., LAMBERT P. Comparison between principal component analysis and independent component analysis in electroencephalograms modeling. Biometrical Journal 49(2): 312-327. **2007**.
- RITTER C., GILLIARD G. ImpuR: A collection of diagnostic tools developed in R in the context of peak impurity detection in HPLC-DAD but potentially useful with other types of time-intensity matrices. Journal of Statistical Software 18(9): 1-18. **2007**.

Products and Services

- Consulting: the SMCS provides expertise on matter such as data collection and management, choice of the adequate statistical methods and use of statistical software.
- Training: the SMCS organises recurrent or on-demand courses about statistical methods or software. Besides our regular training, we may provide customised training.
- Documenting: the SMCS provides statistical documentation and follow-up of the software market and the statistical tools.
- Networking: the SMCS continuously builds a network of statistical experts and maintains active contacts with them to stimulate interdisciplinary collaborations.

Keywords

Statistics
Modelling
Analysis
Consulting
Methodology

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Lightweight metallic and composites structures for efficient transportation

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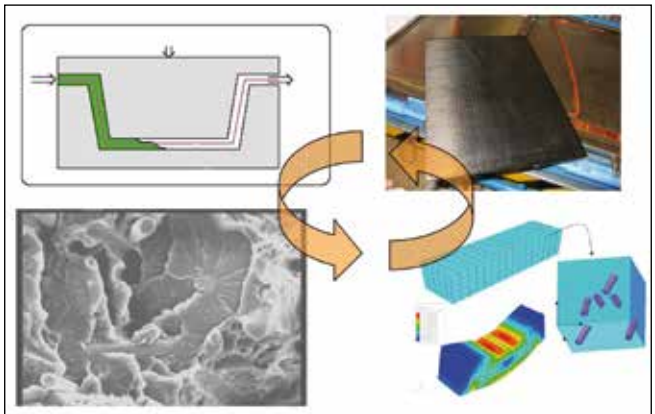
Research Field and Subjects



General research procedure, from materials processing to characterisation, test and modelling

The continuous increase of fuel costs and ever stricter safety standards are the major driving forces for efforts to reduce the weight and increase the reliability of transport vehicles, especially in the airplane and car industries. In recent years, UCL researchers in two institutes (the Institute of Mechanics and Civil Engineering, iMMC, and the Institute of Condensed Matter and Nanoscience, IMCN) have built integrated expertise and capability on lightweight composite materials, metal alloys (steel, Al, Ti) and complex architectured materials. A major research focus is the improvement of toughness, but additional performance is also addressed, depending on the application, *e.g.* durability, fire and thermal management and process integration. The integrated methodology illustrated in the figure involves all steps from processing, characterisation and testing to modelling and simulation with emphasis on a multi-scale approach. Some key capabilities are briefly described below:

- Design and processing of advanced high strength steels, titanium and aluminium alloys. Heat treatments and forming operations (such as hot rolling) to optimise performance;
- Thermoset composites processing encompassing Resin Transfer Moulding (RTM), Same Qualified Resin Transfer Moulding (SQRTM) and Resin Infusion;
- A broad range of physico-chemical, thermal and morphological analysis techniques suitable for composites and metals, in particular IR/Raman spectroscopy, DSC, TGA, DMA, rheology, XRD, OM, SEM, EBSD, TEM, AFM;
- Integrated mechanical testing from nano- to macroscale: nano-indentation, nanoscratch, tension, compression, bending, impact, fracture mechanics (static and fatigue) and delamination, all with ageing, humidity and temperature control. Macromechanical tests performed by the LEMSC laboratory are ISO17025 certified;
- Development of micromechanics-based models for the deformation and damage of metallic or polymeric phases. Digital modelling capability including finite elements analysis and homogenisation methods.

The research is mainly carried out in the framework of Wallonia SKYWIN and GREENWIN projects, European projects and industrial bilateral contracts.

Representative References

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- MARTELEUR M., SUN F., GLORIANT T., VERMAUT P., JACQUES P.J., PRIMA F. On the design of new β-metastable titanium alloys with improved work hardening rate thanks to simultaneous TRIP and TWIP effects. Scripta Materialia 66(10): 749-752. **2012**.
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Funding

▸ Service Public de Wallonie (SPW), Plan Marshall

Partnership

▸ Close collaboration with the Walloon research centers CENAERO and CERTECH (Belgium)
▸ Close collaborations with industry: SONACA, TechspaceAero, SABCA, APERAM
▸ Long term partnership with ArcelorMittal

Main Equipment

▸ Processing (main): High shear extruder (Krupp WPZSK25), DSM Xplore 1 microcompounder with Fiber Spin Line and Micro Film Device, Isojet Equipment RTM, Radius Engineering SQRTM
▸ Thermal analyses: Mettler Toledo DSC/ADSC821e, HP-DSC 827e, TMA 40, Flash DSC1, DMA/SDTA 861e, TGA/SDTA 851e coupled to Thermo Scientific FT-IR Nexus 870
▸ Rheometry: TA ARES with EVF extensional fixture, Paar Physica MC300, Malvern Kinexus with UV curing accessor
▸ Mechanical testing: 10 universal testing machines (up to 1000 kN – 5 static and 5 hydraulic – one with tension-torsion capability) equipped furnaces, micro-tension in SEM, Nanoindentor Agilent, impactor, delamination tests, test fixtures for most normalised tests on composite coupons
▸ Morphology: FEG-SEM (Zeiss Supra55) with EBSD, FEG-SEM (Zeiss Ultra 55) with EDX, TEM (CM-30), XRD (Bruker D8)

Products and Services

▸ Broad range of services and analyses ranging from single tests to full collaborative research projects

Keywords
Polymers
Composites
High strength and lightweight metals and alloys
Mechanical properties
Micromechanics
Characterisation
Multiscale modelling

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High performance lithium-ion batteries

SENIOR SCIENTISTS

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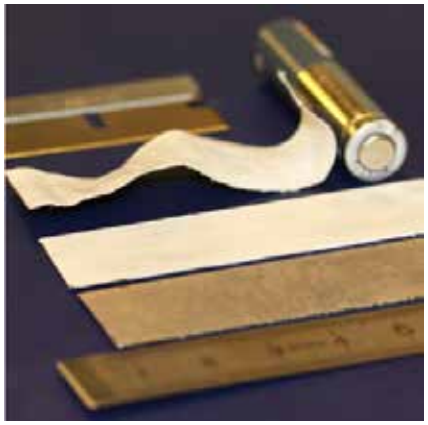
- Sorin MELINTE

Research Field and Subjects



High specific energy, high power density, long cycle life, low cost and safer systems are required for the next generation of Li-ion batteries with numerous targeted applications such as powering of electric vehicles, nomad devices, etc. Current Li-ion batteries have the highest energy density, but they suffer from low power density. Another concern is the requirement for flexible and/or miniaturised Li-ion batteries that can easily be handled and fabricated directly on various substrates. In this framework, we are currently developing new materials for the three basic compartments of a Li-ion battery: the anode, the cathode and the electrolyte separator. Typical examples of our recent achievements are detailed below.

As anode architecture, we develop vertically aligned semiconductor nanowires entrapped in a polymer matrix that operates both as Li^+ gel-electrolyte and electrode separator and gives the batteries good mechanical stability and flexibility. Enhanced performance is obtained by applying porous, electrically interconnected copper shells to the silicon nanowires. This improved performance is now being demonstrated for novel scaffolds built from different types of nano-objects and soft materials.

Work is also being carried out on the development of novel cathode materials based on organic stable radical polymers. More specifically, we develop block copolymers containing a poly(2,2,6,6-tetramethylpiperidinyloxy-4-yl-methacrylate) (PTMA) block. PTMA displays rapid electron transfer kinetics resulting in the high power capability (*i.e.* fast charge-discharge process) of these materials. Other types of organic materials combining the features of conducting and redox-active polymers are also currently being developed.

Novel types of electrolytes based on block copolymers have been fully developed. The nanostructuration process of those systems leads to unique properties including good mechanical properties and ionic conductivity, as well as simple treatment.

Finally, we develop original solutions to handle the different components of batteries (cathode, electrolyte and anode) as inks or paints in which the required ingredients (binders, additives, current collectors) are also incorporated. This allows us to obtain paintable batteries suitable for a variety of supports.

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Funding

- Service Public de Wallonie (SPW), Direction Générale Opérationnelle de l'Economie, de l'Emploi et de la Recherche (DGO6), Direction Générale Opérationnelle Aménagement du territoire, Logement, Patrimoine et Energie (DGO4)
- Fonds de la Recherche Scientifique (F.R.S.–FNRS)

Partnership

- Université de Mons (UMONS) (Belgium)
- Université de Liège (ULg) (Belgium)
- Rice University (USA)

Main Equipment

- Equipment for Li-ion battery nanoarchitectonics and design of components on unconventional substrates
- Basic equipments for battery assembly
- Full electrochemical characterisation of batteries

Products and Services

- Nanostructured semiconductor materials
- Design and prototyping of flexible Li-ion batteries
- Electrochemical characterisation of batteries and standard battery testing

Keywords

Flexible Li-ion batteries
Paintable batteries
Nanostructured anodes and cathodes
Nanoarchitectured current collectors
Organic batteries

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Thin films and nanostructures for photovoltaics

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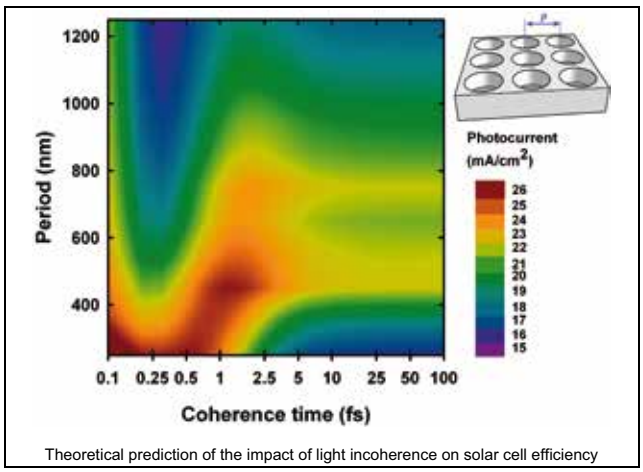
- Jean-Jacques PIREAUX
- Robert SPORKEN
- Guy TERWAGNE
- Jean-Pol VIGNERON †

Research Field and Subjects



Theoretical prediction of the impact of light incoherence on solar cell efficiency

The research topics currently under investigation in our group concern thin-film solar cells, based on crystalline silicon (c-Si), compound semiconductors and Si/Ge quantum dots. Photonic studies deal with angular and spectral broadband trapping of solar light inside corrugated films. Digital simulations are used to predict the best parameters of the front side and/or back side corrugations in order to promote light trapping. These design strategies are applied to ultrathin (a few μm thickness) c-Si solar cell prototypes. Effects of the short coherence time of solar light on the efficiency are theoretically studied (see illustration). On the experimental side, thin films of CZTS(Se) (deposited either by DC/RF sputtering or co-evaporation) are studied, as well as new compound semiconductors, based on low cost, widely available and non-toxic elements. Different methods for introducing the chalcogenide elements are investigated. The same physical deposition methods are used to prepare a new type of transparent conducting oxide (TCO) based on ZnO doped with Al. Optical absorption and electrical characteristics of these TCOs are optimised. Thin films of CIGS on metal substrates are fabricated. The main challenge is to develop diffusion and electrical coating barriers up to 550 °C. For this purpose, vacuum and wet-based processed dielectric coatings are studied with emphasis on polymer-derived ceramic precursors. Surface/interface analyses of various layers are carried out to evaluate adhesive properties. Optimisation of molybdenum coatings used as back contact and fabrication of complete CIGS cells are also investigated. Si and Ge nanoparticles are synthesised by ion implantation in fused quartz as well as in an oxide layer to exploit the increase in efficiency due to multiple excitons generation in quantum dots. After annealing between 900 and 1100°C, Ge-Ge, Si-Ge and Si-Si nanoparticles are formed preferentially at the SiO_2/Si interface. Finally, a biomimetic approach is followed in order to develop novel antireflection and self-cleaning coatings for solar cell panels. The fundamental understanding of the role of natural nanostructure features on antireflective or self-cleaning properties is exploited to develop bio-inspired coatings.

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Patent

▸ Process for the production of photovoltaic cells. WO 2012/028738 (A1), 2012 (Application number WO 2011/EP65255, 2011; Priority numbers US 2010/0380592P, 2010 – EP 2010/0175311, 2010).

Funding

▸ European Commission: 7th Framework Programme
▸ Service Public de Wallonie (SPW): Programme Greenomat, Plan Marshall 2.vert
▸ Wallonie-Bruxelles International (WBI): Coopération Wallonie-Bruxelles/Québec 2013-2015

Partnership

▸ Interuniversity Microelectronics Centre (IMEC) Leuven (Belgium)
▸ CRM Group (Belgium)
▸ Institut des Nanotechnologies de Lyon (INL) (France)
▸ Institut National de la Recherche Scientifique - Centre Energie Matériaux Communication (INRS-EMT) (Canada)
▸ Université catholique de Louvain (UCL) (Belgium)
▸ Université de Mons (UMONS) (Belgium)
▸ Centre Spatial de Liège (CSL) (Belgium)
▸ Materia Nova (Belgium)
▸ AGC Flat Glass Europe
▸ Solvay
▸ LASEA
▸ CET
▸ TAIPRO Engineering

Main Equipment

▸ High performance computing environment with the Interuniversity Scientific Computing Facilities (ISCF)
▸ Optical measurements (spectrophotometry)
▸ Ionolumiscence, photoluminescence
▸ DC/RF sputtering, thermal co-evaporation
▸ X-Ray photoelectron spectroscopy, Time-of-Flight Secondary Ion Mass Spectrometry, DRX, SEM and HR-TEM
▸ RBS, NRA, ERDA, PIGE, PIXE, material analysis using ion beam (accelerators)

Products and Services

▸ Design, synthesis and optimisation of thin film solar cell structures

Keywords

Thin films
Solar cells
Nanostructures
Nanodots
Photonics

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Stimuli-responsive and self-healing supramolecular materials

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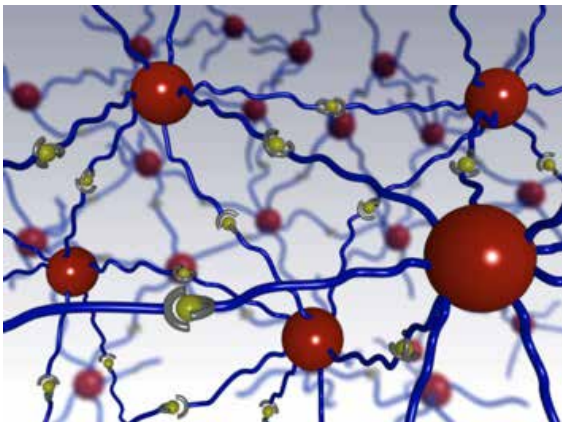
- Evelyne VAN RUYMBEKE

Research Field and Subjects



New materials that have the ability to adapt reversibly to changes in their environment and possess properties such as self-healing, thixotropy, etc. are highly sought after. A promising way to design such materials is to exploit supramolecular interactions which are dynamic and reversible by nature.

This research topic deals with the development of highly tuneable materials by combining polymers with supramolecular interactions, and in particular coordinative metal-ligand bonds. The dynamics of such systems are then studied and modelled to enable the design of smart materials with the desired flow properties. The team has expertise in the synthesis and rheology of functionalised (co)polymers bearing ligands at selected and well-defined locations. The synthesis can be performed by direct polymerisation of functional monomers through controlled radical polymerisation methods (RAFT, ATRP, NMP) or by post-functionalisation of the polymer. Addition of metal ions to these polymers reversibly links the polymer chains in different ways depending on the polymer architecture and location of the ligands, leading to networks, chain extension, etc. In-depth rheological characterisations in the melting and solution of the obtained materials are performed, in shear or extensional flow. Specific properties such as aging, thixotropy, or shear thickening are investigated. The response of these materials to various stimuli (temperature, pH, mechanical stress, competitive binders, etc.) is also studied. For entangled supramolecular polymers, a mesoscopic model based on the tube theory can be applied in order to relate their composition to their linear viscoelastic response.

As an example of realisation stimuli-responsive gels have been obtained by linking together block copolymer micelles, decorated with terpyridine ligands, by metal-ligand bonds. These gels exhibit a rapid self-healing ability, recovering their initial rheological properties in a few seconds only.

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Funding

- Fédération Wallonie-Bruxelles: Action de Recherche Concertée (ARC)
- European Commission: 7th Framework Programme

Main Equipment

- Dynamic and static light scattering (Malvern-ALV CGS-3 and Vasco system Cordouan Technologies)
- GPC system (PSS) with triple detection (DRI, UV diode array, MALS)
- Rheometers ARES, PAAR, Kinexus

Products and Services

- Synthesis of (functionalised) block copolymers by controlled radical polymerisation methods
- Rheological characterisation of polymer melts and solutions
- Modelling of the linear viscoelastic properties of engangled supramolecular homopolymers

Keywords

Gels
Rheology
Metal-ligand bond
Block copolymers
Stimuli responsive materials
Tube modelling

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The behaviour of building material in transient climatic conditions

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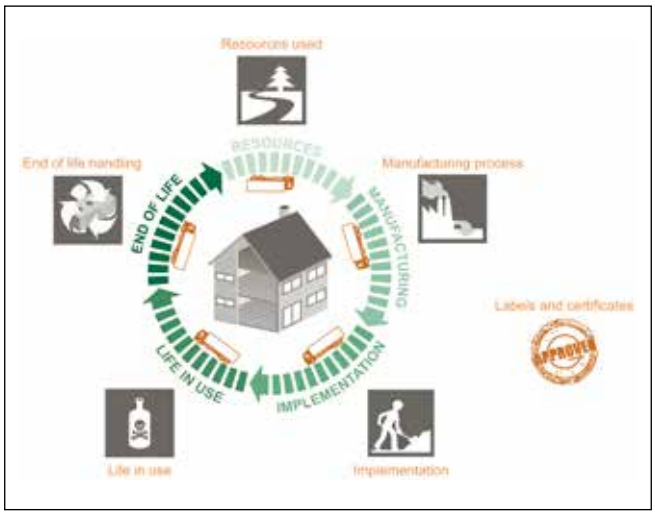
Research Field and Subjects



Researchers focus on building materials with an attractive life cycle to apply bioclimatic and sustainable principles in architectural practice more efficiently. Impacts on global energy demand, comfort or non-desirable effects on health or environments are the guiding features.

Precise criteria are defined to help architects and designers choose materials for housing, service industry buildings or heritage buildings. Those criteria are linked with different strategies to allow integration of the multi-dimensional contexts that architecture has to deal with. Specific topics are highlighted from the materials point of view: thermal inertia, thermal comfort, day lighting, Inside Air Quality (IAQ), moisture regulation, etc.

Bioclimatic "hot" and "cold" strategies have proven to be a useful tool from the first step of building conception and establishment to the last phase of this process where building equipment and finishing materials are chosen. The presumed global energy performances of the building can then be assessed quite precisely with computer modelling, taking into account all the energy savings obtained by passive means together with the optimisation of heating, ventilation and insulation systems. Heat Air and Moisture (HAM) calculations models and computer possibilities are in constant evolution and each development allows greater understanding and control of the global building response to transient climatic conditions. Improving the global performance of buildings is closely linked to the knowledge of materials properties and attention is paid to improving the knowledge of hygroscopic and capillary materials such as lime-hemp concrete, earth mixture, straw bale, etc.

The use of tools and databases to assess the life cycle of materials, components and buildings is another important research field. Global forms of environmental impact are analysed in terms of operational and embodied energy, as well as in terms of Green House Gas (GHG) emissions and many other criteria, taking account of transport and health through each step of the life cycle.

Representative References

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Award

- Belgian Price for Energy and Environment, Category "Education Eco-Award 2010" (A. De Herde)

Funding

- Regions (Wallonia, Brussels, Flanders)
- Federal State
- European Union (EU)
- Industry

Partnership

- Fédération de l'Industrie Cimentière belge (FEBELCEM) (Belgium)
- Lhoist R&D, Nivelles (Belgium)
- Fraunhofer-Institut für Bauphysik, Holzkirchen (Germany)
- Universität Siegen (Germany)
- Université de Genève (Switzerland)
- University of London (United Kingdom)
- Toegepast-Natuurwetenschappelijk Onderzoek (TNO), Eindhoven (the Netherlands)
- Sapienza - Università di Roma (Italy)

Main Equipment

- Powerful computer device with appropriate software license are the main tool of the research center. Partnership with universities or independent laboratories offers results from measurements that combine perfectly with the computer simulations.

Products and Services

- Several guides for architects and designers are published under specific features where the influence of choosing one material or another is discussed.
- Numerous energetic audits are also realised every year and they enhance building material influences.

Keywords

Bioclimatic
Comfort
Modelling
Insulation
Life cycle
Moisture
Sustainable
Transient

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Carbon-based solids prepared by molecular strategies

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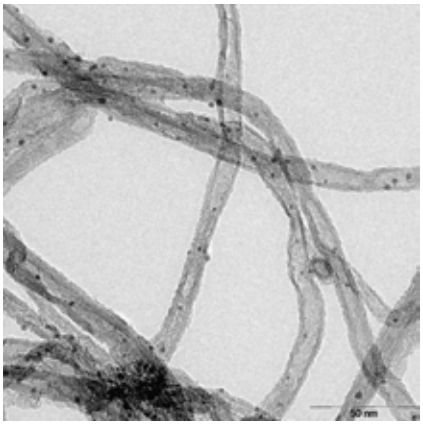
Research Field and Subjects



Molecular approaches are being developed for the modification of solid carbon materials. These range from activated carbon to graphene and include carbon nanotubes and nanofibers. Three main strategies are used to introduce chemical functionalities at the surface of carbonaceous solids: (i) oxidation, (ii) covalent functionalisation by radicals, (iii) non-covalent functionalisation using pi-pi interactions. In the first case, oxygenated groups are introduced at defect sites and can be used for the direct grafting of metal complexes by ligand exchange. Inorganic complexes presenting carboxylate ligands are particularly suited for such ligand exchange, leading to covalently grafted metal-containing moieties. In the second case, new families of radicals are being explored, and in particular xanthates in conjunction with radical initiators. This allows for the functionalisation of carbon nanotubes sidewall with a high density of highly variable chemical functions, for instance activated esters, protected amines, etc. The same methodology is applicable to reduced graphene oxide (rGO). Bifunctional carbon surfaces are obtained by grafting both halves of the starting xanthate or using modified initiators. In the third case, pyrene derivatives are coupled to the properties-bearer group of interest and introduced on the carbon support in one step. Catalytically active complexes can thus be immobilised in one step with no prior attack of the carbon structure. This is highly advantageous to obtain single-site materials and/or to avoid losing some of the exceptional properties of the starting nano-carbon.

The main application that has been explored so far is the synthesis of carbon-supported nanoparticles by controlled thermal coalescence of the grafted complexes. Our grafting procedure ensures optimal dispersion and small sizes of the final nanoparticles. In parallel, we have immobilised homogeneous catalysts to form heterogenised organometallic complexes that become recyclable.

Representative References

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Funding

▸ Fonds de la Recherche Scientifique (F.R.S.-FNRS)
▸ Belgian National Lottery
▸ Fédération Wallonie-Bruxelles
▸ Fédération Wallonie-Bruxelles: Fonds Spécial de Recherche (FSR) UCL

Partnership

▸ Nanocyl S.A

Main Equipment

▸ Inorganic chemistry lab: gloveboxes, autoclaves, ovens, Schlenk vacuum lines for syntheses under inert atmosphere
▸ Infrared (IR) and Raman spectroscopy with *in situ* cell
▸ Thermogravimetric analyses (TGA-MS)
▸ Textural characterisations (N_2 physi- or chemisorption)
▸ Atomic absorption spectrometry (AA)

Products and Services

▸ Carbon materials functionalisation
▸ Solid materials surface chemistry
▸ Carbon solids characterisation

Keywords
Activated carbon
Carbon
Functionalisation
Nanofibers
Nanoparticles
Nanotubes
Supported catalysts
Surface chemistry

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Oxide-based materials for catalytic applications: preparation, characterisation and performance

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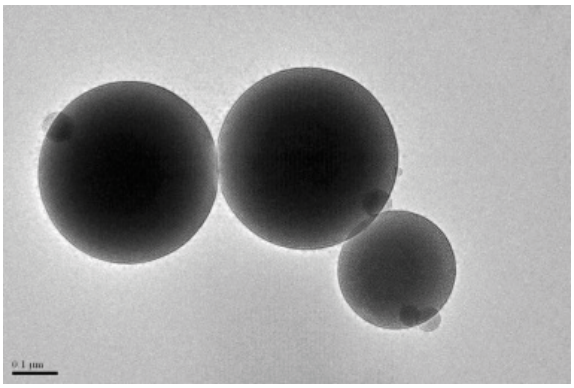
- Eric GAIGNEAUX

Research Field and Subjects



Silica-alumina-molybdena mixed oxide catalyst prepared by the aerosol process.

There is a clear demand for new chemical methods to produce catalytic oxides in various forms: bulk oxides with adequate morphology and textural properties, dispersed supported oxides or thin films. UCL masters the classical procedures (impregnation, co-precipitation, deposition-precipitation, thermal-spreading, spin-coating) and develops non-conventional approaches using molecular precursors, organic-inorganic hybrids and modified sol-gel chemistry. The aim is to prepare materials with dimensional features in the nanometer-range.

Stoichiometrically well-defined Nb/M coordination compounds (oxo- or peroxo-complexes with (polyamino-)carboxylate ligands) are developed as molecular precursors for Nb-M mixed oxides (M = V, Mo, Ta, Y, Bi) that were stabilised under moderate conditions. Homogeneous V-Mo-Ti, W or Mo or Re-Al-Si xerogels are prepared in one-pot via non-hydrolytic sol-gel, yielding highly dispersed surface species. Similar formulations are obtained by the aerosol process, taking advantage of the fast evaporation-induced self-assembly of templating molecules to generate mesostructured mixed oxide catalysts.

M-M' oxides are prepared from inorganic-organic hybrids in which ampholytic copolymers are used as matrices to stabilise inorganic species (metal ions, complexes or coordination compounds). This route allows the preparing of oxides as Bi vanadates, Nb tantalates, Nb, Co and Ni molybdates, etc. The supra-molecularity and the hydrophobi-hydrophilicity balance of the copolymer confer on the final oxides an unusual texture, crystalline phases and catalytic behaviour.

Oxide thin films with thicknesses in the range of a few to a few hundred nanometers are coated on steel, glass and polymers to give these substrates (photo)-catalytic, optical, stimuli-responsive and luminescent properties. UCL is able to control their thickness, composition, homogeneity, hydrophobic-hydrophilic balance, crystallinity and porosity.

Representative References

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▸ GANNOUN C., DELAIGLE R., ELOY P., DEBECKER D.P., GHORBEL A., GAIGNEAUX E.M. Sol–gel derived V_2O_5–TiO_2 mesoporous materials as catalysts for the total oxidation of chlorobenzene. Catalysis Communications 15: 1-5. **2011**.

Patents

▸ Method of olefin metathesis using a catalyst based on a spherical material comprising oxidized metal particles trapped in a mesostructured matrix. WO 2013/011209 (A1), 2013 Application number WO 2012/FR00285, 2012; Priority number FR 2011/0002221, 2011).
▸ Method of carrying out CC-coupling reactions using oxide supported Pd-catalysts. WO 2013/004814 (A1), 2013 (Application number WO 2012/EP63238, 2012; Priority number EP 2011/0173056, 2011).
▸ Functional multilayer system. WO 2013/164255 (A1), 2013 (Application number WO 2013/EP58668, 2013; Priority number EP 2012/0166155, 2012).

Awards

▸ Prix Triennal de la Société Royale de Chimie 2013 (E. Gaigneaux)
▸ Prix de la Société de Chimie Industrielle – Branche belge 2012 (D. Debecker)
▸ Umicore Scientific Award 2010 (D. Debecker)
▸ Exxon Mobil European Award 2003 (E. Gaigneaux)

Funding

▸ Belgian Science Policy Office (BELSPO): Interuniversity Attraction Pole (IAP)
▸ Service Public de Wallonie (SPW): Direction Générale Opérationnelle de l'Economie, de l'Emploi et de la Recherche (DGO6)
▸ Fonds de la Recherche Scientifique (F.R.S.-FNRS)
▸ Fédération Wallonie-Bruxelles: Fonds Spécial de Recherche (FSR) UCL

Partnership

▸ Université de Montpellier, Institut Charles Gerhardt Montpellier, Pr H. Mutin (France)
▸ Université Pierre et Marie Curie, Laboratoire de Chimie de la Matière Condensée de Paris, Pr C. Sanchez (France)
▸ Université de Namur (UNamur), Laboratoire de Physique du Solide, Pr J.-P. Vigneron and Pr O. Deparis (Belgium)
▸ Université de Mons (UMONS), Laboratoire de Physique des Surfaces et Interfaces, Pr J. De Coninck (Belgium)
▸ Université de Liège (ULg), Groupe de Recherche en Energie et ENvironnement à partir des MATériaux (GREEnMat), Laboratoire de Chimie Inorganique Structurale (LCIS), Pr R. Cloots and Pr B. Vertruyen (Belgium)

Main Equipment

▸ Equipment for preparation and shaping of oxide based catalysts at lab and pilot scales
▸ Reactors for gas and liquid phase catalysis: total oxidation (of air pollutants), partial oxidation, dehydrogenation, metathesis amm- and epoxidation, acid-base (trans)esterification and dehydration
▸ Infrared and Raman *in situ* (and *operando*) spectroscopy
▸ Thermogravimetric analysis – Differential Scanning Calorimetry (TGA-DSC)
▸ Physi- and chemisorption of gas (textural properties, acido-basicity and redox measurements)
▸ X-ray (thermo) diffraction and X-ray photoelectron spectroscopy for particle size and surface analysis
▸ Electron and optical microscopies
▸ Equipment for preparation and cleaning of films (spin-coating, ozone chamber, clean furnaces)
▸ Measurement of hydrophobic-hydrophilic balance by contact angle

Products and Services

▸ Catalysts preparation (including at the pilot scale, and shaping) and characterisation
▸ Measurement of performance in dedicated catalytic reactions

Keywords

Air depollution
Dehydration
Epoxidation
Mixed oxides
Oxide catalysts
Oxidation
Oxidative dehydrogenation
Supported oxides

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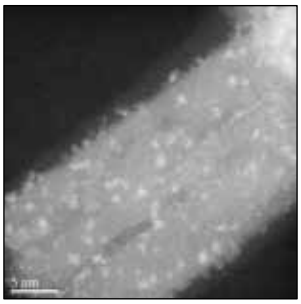
Metal-based materials for catalytic applications: preparation, characterisation and performance

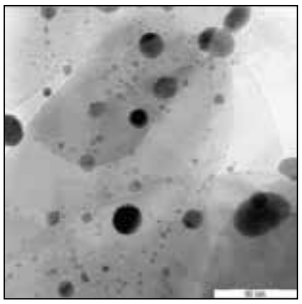
SENIOR SCIENTISTS

- Damien DEBECKER
- Michel DEVILLERS
- Eric GAIGNEAUX
- Sophie HERMANS

Research Field and Subject



Transmission electron micrograph of palladium supported on boron nitride catalyst active in lactose oxidation



Transmission electron micrograph of rutile TiO_2 nanorod (grey) loaded with Ru nanoparticles (brighter) for the methanation of CO_2.

Numerous heterogeneous catalysts have their active species consisting of small quantities of metal, including noble metals, deposited on oxides or carbon supports. "Supported" metals might be in the form of nanoparticles, clusters or isolated atoms, all exhibiting a high dispersion, *i.e.* a high proportion of exposed, and thus active, metal atoms. "Supporting" metals also allows stabilising the metals in their most efficient form and/or providing them with resistance to sintering.

Thanks to its knowledge of a large variety of metal deposition methods, the team has the capability to control the state of supported metal catalysts in terms of location of the metal inside or outside the porosity of the support, its dispersion, crystallinity and particle size, the nature of the metal species, the type of interaction with the support, etc. The team is also well-equipped to characterise physico-chemical properties of metal based catalysts and is able to measure their catalytic performance in numerous chemical reactions both in liquid or gas phases.

As an example, supported nanoparticle catalysts are developed for carbohydrate conversions in the liquid phase. Pd-based formulations are synthesised using molecular precursors. The synthetic methodology involves optimising the precursor/support surface interactions. This is implemented using various strategies such as modulating surface charge and precursor species to favour electrostatic interactions; this functionalises the support to allow grafting procedures, using physical parameters such as solvent dielectric constant to optimise the impregnation step. Supports such as carbon, oxides and boron nitride are investigated. Bimetallic catalysts prepared from single-source molecular precursors are also studied for synergetic effects.

Similar examples concerning pharmaceutical catalysis (C-C coupling), air depollution (VOC abatement), hydrogenation of N_2 to NH_3, methanation of CO_2, etc. also deserve to be mentioned.

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- HERMANS S., DEFFERNEZ A., DEVILLERS M. Au-Pd/C catalysts for glyoxal and glucose selective oxidations. Applied Catalysis A: General 395(1-2): 19-27. **2011**.
- WOJCIESZAK R., GENET M.J., ELOY P., RUIZ P., GAIGNEAUX E.M. Determination of the size of supported Pd nanoparticles by X-ray photoelectron spectroscopy. Comparison with X-ray diffraction, transmission electron microscopy, and H_2 chemisorption methods. The Journal of Physical Chemistry C 114(39): 16677-16684. **2010**.

Awards

- Prix Triennal de la Société Royale de Chimie 2013 (E. Gaigneaux)
- Prix de la Société de Chimie Industrielle – Branche belge 2012 (D. Debecker)
- Umicore Scientific Award 2010 (D. Debecker)
- Exxon Mobil European Award 2003 (E. Gaigneaux)

Funding

- Fonds de la Recherche Scientifique (F.R.S.-FNRS)
- Belgian Science Policy Office (BELSPO): Interuniversity Attraction Pole (IAP)
- Fédération Wallonie-Bruxelles: Fonds Spécial de Recherche (FSR) UCL
- Service Public de Wallonie (SPW), Direction Générale Opérationnelle de l'Economie, de l'Emploi et de la Recherche (DGO6)

Partnership

- Université Pierre et Marie Curie, Collège de France, Laboratoire Chimie de la Matière Condensée de Paris, Pr C. Sanchez (France)

Main Equipment

- Equipment for preparation and shaping of metal based catalysts at lab and pilot scales
- Versatile reactors for gas and liquid phase catalysis
- Infrared and Raman *in situ* spectroscopy
- ATG-MS, DSC
- Physi- and chemisorption of gas (textural properties, metal dispersion measurements)
- X-ray diffraction and X-ray photoelectron spectroscopy for particle size and surface analysis
- Electron microscopies

Products and Services

- Catalysts preparation and characterisation
- Measurement of catalytic performance in dedicated catalytic reactions

Keywords

Air depollution
Carbohydrates
Carbon
Fine chemistry
Hydrogenation
Nanoparticles
Oxidation
Supported catalysts

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Scaling up, shaping and structuration of catalytic materials

SENIOR SCIENTISTS

- Damien DEBECKER
- Eric GAIGNEAUX

Research Field and Subjects

Scaling-up and structuration tools available at UCL: 150 L precipitation vessel (left), extrusion (up right), pelletization (bottom right).

A macroscopic silica monolith with hierarchical porosity (left), powders and honeycomb monoliths and extrudates (middle), pellets.

Our research group is able to prepare catalytic materials on a large scale. This includes:

- The scaling up of catalyst preparation from the gramme scale to several kilogrammes;
- The structuration of powder catalysts as pellets, extrudates or monoliths;
- The direct shaping of monolith catalyst via sol-gel. All kinds of inorganic materials (excluding alloys) are involved, mostly supports, including carbon-based materials, zeolites, oxide materials, and encapsulated or supported catalysts derived from these.

Gas phase catalytic applications in the field of the environment (*e.g.* air and gas exhaust depollution) and energy production (*e.g.* catalytic burners) are inevitably associated with high flow rates. Structuration into pellets, extrudates or monoliths is the only way to avoid pressure drops. Likewise in fine chemistry (including pharmaceutical), oleochemistry, etc., there is a strong trend to switch from batch to flow production processes. This requires the use of heterogeneous macroscopic catalysts in which diffusion constraints are properly addressed.

Moreover, in academia, developments of catalyst formulations and preparations are made at the gramme scale. Implementation of academic recipes in industry requires a validation at the pilot kilogramme scale. This applies to catalysts but also to inorganic absorbants, adsorbants, ceramic precursors, pigments, etc. Mastering scaling-up aspects is actually key to the transfer of academic findings to the industry.

One sort of structured catalyst consists of catalytically active powders anchored on rigid macroscopic supports, typically metal fibres or plates, metallic or ceramic monoliths with an open honeycomb-like structure. The overall structured catalysts thus exhibit both the catalytic efficiency of the anchored powders and the physical properties of the supports, *e.g.* low-pressure drop. Alternatives are to shape the catalytic powders in the form of macroscopic bodies, and the direct preparation of porous materials of the desired macroscopic shape (beads, monoliths) presenting hierarchical porosity (macro, meso, micro) and physical resistance. This strategy is developed by a one-step sol-gel method. The solids are either used directly as catalysts (active components introduced during the preparation) or serve as supports for the anchoring of other active species.

Representative References

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- BALDOVINO-MEDRANO V.G., FARIN B., GAIGNEAUX E.M. Establishing the role of graphite as a shaping agent of vanadium-aluminium mixed (hydr)oxides on their physicochemical properties and catalytic functionalities. ACS Catalysis 2(3): 322-336. **2012**.
- BALDOVINO-MEDRANO V.G., LE M.T., VAN DRIESSCHE I., BRUNEEL E., GAIGNEAUX E.M. Influence of graphite as a shaping agent of Bi molybdate powders on their mechanical, physicochemical and catalytic properties. Industrial & Engineering Chemistry Research 50(9): 5467-5477. **2011**.

Patent

- Procédé de préparation de monolithes silico-aluminiques macroporeux, monolithes silico-aluminiques macroporeux obtenus selon ce procédé, et leur utilisation à titre de catalyseur acide, filed. FR 1257233, 2012.

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- Fonds de la Recherche Scientifique (F.R.S.-FNRS)
- Fédération Wallonie-Bruxelles: Fonds Spécial de Recherche (FSR) UCL
- European Commission: 7th Framework Programme, Marie Curie Actions

Partnership

- Université de Bordeaux 1, Centre de Recherches Paul Pascal, Pr R. Backov (France)
- Université Pierre et Marie Curie, Laboratoire de Chimie de la Matière Condensée de Paris, Pr C. Sanchez (France)

Main Equipment

- Equipment for preparation of structured catalysts, and shaping of catalytic powders at pilot scale : 150L vessel, 25L rotating evaporator, 1L-Soxhlet, continuous 0.1 m^2 filter, 3L-rotating furnace, malaxing blender, extruder, automated pelletisation machine
- Reactors for gas and liquid phase catalysis
- Spectroscopes, microscopes and other physicochemical equipments to characterise the texture, the structure and surface properties and composition of inorganic (catalytic) solids

Products and Services

- Scaling-up of synthesis protocols of inorganic (catalytic) solids
- Shaping, extrusion, pelletisation or structuration
- Characterisation of inorganic materials and catalytic activity measurements

Keywords

Extrusion
Flow reaction
Monolith
Pelletisation
Pilot scale
Scaling-up
Sol-gel
Structuration

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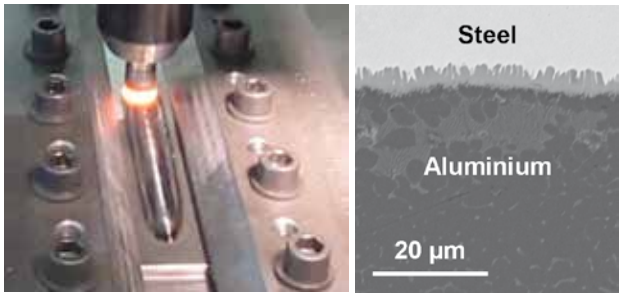
Innovative joining of materials: friction stir welding and adhesive bonding

SENIOR SCIENTISTS

- Francis DELANNAY
- Bruno DE MEESTER
- Vincent DESTOOP
- Pascal JACQUES
- Frédéric LANI
- Thomas PARDOEN
- Aude SIMAR

Research Field and Subjects



Two major research activities of the Institute of Mechanics, Materials and Civil Engineering (iMMC) concern innovative assemblies: friction stir based processes and adhesive bonding.

Friction Stir Welding (FSW) is a novel fully automated solid-state process. A rotating tool is forced down into the material producing frictional heating to temperature at which it is easily plasticised and stirred. This process eliminates defects inherent to fusion welding processes (porosity, solidification cracking, etc.). In iMMC, a large variety of alloys have been successfully welded (aluminium, magnesium and copper alloys) in similar or dissimilar welding configurations.

A new patented friction stir based process enables the welding of dissimilar metals presenting large differences in fusion temperature such as aluminium alloys to steel (see image above).

Current research in welding is concerned with:

- Optimisation of the welding process parameters;
- Modelling of the thermo-mechanical cycles during FSW;
- Characterising and understanding the evolutions of microstructures;
- Predicting the global structural behaviour of welds.

The research strategy relies on a multi-physics and multi-scale approach.

Adhesive bonding is increasingly used in many industrial fields owing to its numerous advantages (lightness, insulation, versatility, etc). Nevertheless, the mechanical resistance and durability remain key issues for applications in primary structural components. For more than 15 years UCL has carried out both fundamental and applied research to set up a combined experimental and modelling strategy in order to predict the mechanical reliability of bonded coupons and structures. Recently (see references), a new approach for predicting fracture in adhesive joints has been proposed and successfully assessed for a variety of adhesives and loading conditions. The most recent study aims at designing adhesive joints to improve the failure resistance in the context of an FP7 research project (BOPACS).

Representative References

- JONCKHEERE C., DE MEESTER B., DENQUIN A., SIMAR A. Torque, temperature and hardening precipitation evolution in dissimilar friction stir welds between 6061-T6 and 2014-T6 aluminum alloys. Journal of Materials Processing Technology 213(6): 826-837. **2013**.
- SIMAR A., BRECHET Y., DE MEESTER B., DENQUIN A., GALLAIS C., PARDOEN T. Integrated modelling of friction stir welding of 6XXX series aluminium alloys: process, microstructure and properties. Progress in Materials Science 57(1): 95-183. **2012**.
- MARTINY P.H., LANI F., KINLOCH A.J., PARDOEN T. A maximum stress at a distance criterion for the prediction of crack propagation in adhesively-bonded joints. Engineering Fracture Mechanics 97(1): 105-135. **2012**.
- MARTINY P.H., LANI F., KINLOCH A.J., PARDOEN T. A multiscale parametric study of mode I fracture in metal-to-metal low-toughness adhesive joints. International Journal of Fracture 173(2): 105-133. **2012**.
- DEPLUS K., SIMAR A., VAN HAVER W., DE MEESTER B. Residual stresses measurements on friction stir welding of aluminium alloys. International Journal of Advanced Manufacturing Technologies 56(5-8): 493–504. **2011**.
- NIELSEN K., PARDOEN T., TVERGAARD V., DE MEESTER B., SIMAR A. Modelling of plastic flow localisation and damage development in friction stir welded 6005A aluminium alloy using physics based strain hardening law. International Journal of Solids and Structures 47(18-19): 2359-2370. **2010**.
- SIMAR A., JONCKHEERE C., DEPLUS K., PARDOEN T., DE MEESTER B. Comparing similar and dissimilar friction stir welds of 2017 – 6005A aluminium alloys. Science and Technology of Welding and Joining 15(3): 254-259. **2010**.

Patent

- Method for welding at least two layers. WO 2013/164294 (A1), 2013 (Application number WO 2013/EP58844, 2013; Priority number EP 2012/0166124, 2012).

Funding

- Belgian Science Policy Office (BELSPO): Interuniversity Attraction Poles (IAP), Technology Attraction Poles – Phases 1 and 2 (TAP2)
- European Commission: 6th and 7th Framework Programmes
- Fonds de la Recherche Scientifique (F.R.S-FNRS)
- Fonds de la Recherche Scientifique (F.R.S-FNRS): Fonds pour la Formation à la Recherche dans l'Industrie et l'Agriculture (FRIA)
- Service Public de Wallonie (SPW), Programme Winnomat

Partnership

- Centre d'Etudes Wallon d'Assemblage et du Contrôle des matériaux (CEWAC) (Belgium)
- Belgian Welding Institute (Belgium)
- Technical University of Denmark (DTU), Dr K.K. Nielsen, Pr V. Tvergaard (Denmark)
- Office National d'Etudes et de Recherches Aérospatiales (ONERA), Dr A. Denquin (France)
- Imperial College London, Pr A.G. Kinloch (United Kingdom)
- Centre d'Excellence en Recherche AEROnautique (CENAERO), Dr. P. Martiny (Belgium)

Main Equipment

- FSW machine fully instrumented for recording torque, forces in the three directions, tool temperatures as well as temperatures in the joint
- Macro-mechanical tests (tension-compression, bending, fracture mechanics tests), micro- or nano-mechanical tests (nano-indentation, *in situ* testing in SEM), adhesion tests under different load mixity for metallic and composites joints, as well as for thin multilayers
- Characterisation methods: optical and electronic microscopy (TEM and SEM), EBSD, x-ray diffraction, metallographic preparation

Products and Services

- Elaboration of assemblies in a fully instrumented environment
- Microstructure and mechanical characterisation of assemblies
- Modelling of the microstructure evolution, mechanical properties and fracture mechanics

Keywords

Friction stir welding
Adhesive bonding
Dissimilar welding
Multiscale modelling
Fracture mechanics
Mechanical properties
Aluminium alloys

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3D molecular characterisation at the sub-micrometer scale

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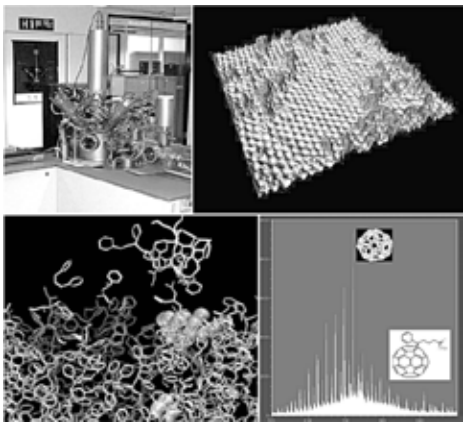
- Sami YUNUS
- Patrick BERTRAND

Research Field and Subjects



The development of new surface treatments and modifications in nano-technologies requires a fine control of the surface molecular composition and structure at the sub-micrometer scale. In terms of characterisation, the main expertise of the group concerns the development and use of surface analytical methods based on ion-solid interaction, in combination with other surface techniques such as XPS and near field microscopy (AFM, STM).

More specifically, for twenty years, the team has been contributing to the development of secondary ion mass spectrometry (SIMS) for the molecular characterisation of surfaces, with a special emphasis on organic materials such as polymers or proteins. The SIMS technique is inherently a nanoscale chemical characterisation technique because of its very limited information depth (~1 nm). Owing to recent developments of the method, including better focusing of ion beams down to 50nm in size, the technique has reached the level required for nanoscale molecular imaging. With the advent of cluster ions sources such as massive noble gas clusters ($Ar_{500-5000}$), sub-micrometric 3D molecular imaging has become possible as the reduced sample degradation induced by these primary ion probes allows the integrity of molecular signals upon depth profiling of the surface to be maintained. The recent experimental progress in cluster-SIMS is also strongly supported by the microscopic modelling activity of the group: here molecular dynamics (MD) simulations are used to understand cluster-surface interactions and predict the behaviour of new projectiles in order to guide future instrumental development.

The application fields of the characterisation methods developed in this group include thin organic films and supramolecular assemblies, biomaterials and hybrid materials, biosensors, organic and molecular electronic devices, catalysts, etc. In addition to the characterisation of samples and materials obtained through collaborations, the group also uses different approaches to modify the surface of materials at the micro- and nanoscales, including chemical and physical treatments: plasma treatments, ion beam irradiation, chemical grafting, conducting polymer film growth, electrochemistry, thin (organic / metallic) layer adsorption, soft lithography and breath figure imprinting.

Representative References

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- MOUHIB T., POLEUNIS C., MOELLERS R., NIEHUIS E., DEFRANCE P., BERTRAND P., DELCORTE A. Organic depth profiling of C_{60} and C_{60}/phtalocyanine layers using argon clusters. Surface and Interface Analysis 45(1): 163-166. **2013**.
- CZERWINSKI B., DELCORTE A. Molecular dynamics study of fullerite cross-linking under keV C_{60} and Ar_n cluster bombardment. The Journal of Physical Chemistry C 117(7): 3595-3604. **2013**.
- RESTREPO O.A., DELCORTE A. Argon cluster sputtering of a hybrid metal-organic surface: A microscopic view. The Journal of Physical Chemistry C 117(6): 1189-1196. **2013**.
- PRABHAKARAN A., YIN J., NYSTEN B., DEGAND H., MORSOMME P., MOUHIB T., YUNUS S., BERTRAND P., DELCORTE A. Metal condensates for low-molecular-weight matrix-free laser desorption/ionization. International Journal of Mass Spectrometry 315: 22-30. **2012**.

Patents

- Membrane for encapsulation chamber of cells producing at least a biologically active substance and bioartificial organ comprising same. WO 02/060409 (A1), 2002 (Application number WO 2002/FR00347, 2002; Priority number FR 2001/0001248, 2001).
- Biomaterial and method for obtaining it. WO 96/15223 (A1), 1996 (Application number WO 1995/BE00104, 1995; Priority number BE 1994/0001022, 1994).

Funding

- Fonds de la Recherche Scientifique (F.R.S.-FNRS)
- European Commission: 7th Framework Programme
- Belgian Science Policy Office (BELSPO): Interuniversity Attraction Poles (IAP)
- Fédération Wallonie-Bruxelles: Action de Recherche Concertée (ARC), Fonds Spécial de Recherche (FSR) UCL
- Service Public de Wallonie (SPW): Direction Générale Opérationnelle de l'Economie, de l'Emploi et de la Recherche (DGO6), Plan Marshall
- Université catholique de Louvain (UCL), Commission pour la Coopération au Développement (CCD)

Partnership

- Other Belgian universities
- Penn State University (USA)
- Université Pierre et Marie Curie) Paris 6 (France)
- Kyoto University (Japan)
- ION-TOF GmbH (Germany)

Main Equipment

- SUrface CHaracterisation platform (SUCH):
  - Secondary Ion Mass Spectrometry: 3 imaging time-of-flight mass spectrometers (ToF-SIMS), including a new instrument with automated 3D imaging capabilities and Ar_n cluster source
  - Scanning Auger Microscopy (AES–SAM)
  - X-Ray Photoelectron Spectroscopy (XPS-ESCA): 2 instruments
- IMCN access to AFM, STM, SEM, TEM, XRD, ellipsometry, static and dynamic contact angles, IR, Raman
- Other access to clean room facilities

Products and Services

- Service provided to companies for practical surface/thin film characterisation and imaging

Keywords

3D molecular imaging
Mass spectrometry
Ion spectrometry
Surface characterisation
Surface modification

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Technology platform: Bio and Soft Matter (BSMA) Polymer materials processing and thermomechanical analysis platform

SENIOR SCIENTISTS

- Christian BAILLY
- Jacques DEVAUX
- Michel SCLAVONS
- Evelyne VAN RUYMBEKE
- Pascal VAN VELTHEM

Research Field and Subjects

The Bio and Soft Matter (BSMA) division of the Research Institute for Condensed Matter and Nanoscience (IMCN) has built polymer processing and thermomechanical characterisation capabilities covering a wide area of research and application areas. Some of the key facilities and corresponding expertise include:

- Thermoplastic compounding and internal mixing at scales from 10 gram to 50 kg/hour. A unique water-assisted extrusion process has been implemented, which has been shown useful for the development of nanocomposites with optimal mechanical and thermal properties.
- Thermoset composite processing by Resin Transfer Moulding (RTM) and Same Qualified Resin Transfer Moulding (SQRTM) intended mainly for the production of high-performance carbon fibre composite panels.
- A full range of thermal analysis instruments and methods, including DSC, modulated DSC, ultrafast "Flash" DSC, TGA, TMA and DMA.
- A full range of rheological instruments and methods, including strain- and stress-controlled rotational rheometry as well as uni-axial extensional rheometry. Specific experimental methods have been developed to cover materials with slow dynamics (creep), curing materials (gel time determination) and coupled methods (rheometry with UV-curing, rheometry with dielectric analysis). Modelling capabilities using "tube theories" are in an advanced stage of development.

These thermomechanical characterisation capabilities are complemented by a broad range of spectroscopic and microscopic methods available through collaboration with other research groups within the IMCN Institute.

Representative References

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- VAN RUYMBEKE E., VLASSOPOULOS D., KAPNISTOS M., LIU C.Y., BAILLY C. Proposal to solve the time-stress discrepancy of tube models. Macromolecules 43(1): 525-531. **2010**.

Patents

- Hybrid material for electromagnetic absorption. WO 2012/032117 (A1), 2012 (Application number WO 2011/EP65554, 2011; Priority number EP 2010/0175887, 2010).
- Process of extruding a polymer in the presence of water. WO 2012/089976 (A1), 2012 (Application number WO 2011/FR53186, 2011; Priority number FR 2010/00061274, 2010).

- Polymer composite material structures comprising carbon based conductive loads. WO 2008/068042 (A2), 2008 (Application number WO 2007/EP10786, 2007; Priority numbers EP 2006/0025002, 2006 – EP 2007/0010440, 2007).

Funding

- Service Public de Wallonie (SPW): Programme Winnomat, Plan Marshall
- European Commission: 7th Framework Programme
- Fédération Wallonie-Bruxelles: Action de Recherche Concertée (ARC)
- Various industrial collaborations

Partnership

- Université catholique de Louvain (UCL): close collaborations within IMCN and with Institute of Mechanics, Materials and Civil Engineering (IMMC)
- Centre de Ressources Technologiques en Chimie (CERTECH)

Main Equipment

- Processing: Brabender plastograph, two-roll mill, extruders Brabender (single & twin screw), high shear extruder (Krupp WPZSK25), injection molding (Krauss-Maffei KM 80-160E), DSM Xplore 1 microcompounder with fiber spin line and micro film device, isojet equipment RTM, radius engineering SQRTM
- Thermal analyses: Mettler Toledo DSC/ADSC821e, HP-DSC 827e, TMA 40, Flash DSC1, DMA/SDTA 861e, TGA/SDTA 851e coupled to thermo scientific FT-IR Nexus 870
- Rheometry: TA ARES with EVF extensional fixture, Paar Physica MC300, Malvern Kinexus with UV curing accessor

Products and Services

- Broad range of services and analyses ranging from single tests to full collaborative research projects

Keywords

Polymers
Composites
Nanocomposites
Processing
Thermal analysis
Rheology

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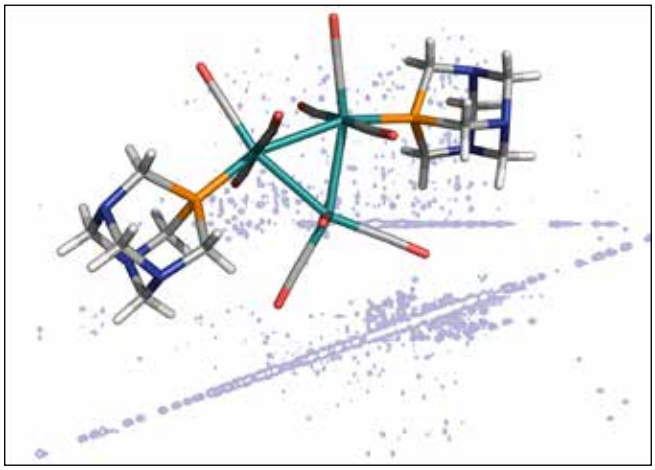
Technology platform: Molecular Structure Analysis (ASM)

SENIOR SCIENTISTS

- Cécile LE DUFF
- Koen ROBEYNS
- Raoul ROZENBERG
- Bernard TINANT

Research Field and Subjects



This Technology Platform unites three complementary techniques and the know-how that permits structural characterisation of small molecules as well as macromolecular systems, namely single crystal X-Ray Diffraction (XRD), liquid–state Nuclear Magnetic Resonance (NMR) and Mass Spectrometry (MS). Our highly qualified team is at hand to identify the best possible technique (or combination of techniques) to address the researchers' problems.

Single crystal X-ray diffraction involves not only the precise determination of atoms but also the ability to detect and characterise polymorphs, study hydrogen bond interactions or for example determine the spin state of Fe-complexes through the Fe-N bond lengths.

In addition to single crystal diffraction, there is the possibility to perform powder diffraction studies in combination with heating/cooling to gain insights in temperature-dependent phase transitions (identification of new compounds, decomposition pathways, phase transformations, etc.).

NMR spectroscopy is an excellent method to determine of molecular conformations or the position of specific moieties in chemical compounds.

For instance, in the field of polymers NMR can help to determine the tacticity (or relative stereochemistry) of polypropylene (PP) using 13C NMR quantitative analysis.

Another example where NMR can be of help to the materials chemist is the study of polyethylene (PE) at high temperatures. PE can be produced using several co-monomers, leading to compounds with different physical properties. The type of co-monomers (qualitative analysis) and their content (*i.e.* the degree of branching – quantitative analysis) can be determined using one-dimensional 13C NMR spectra.

More detailed information on the different types of analyses can be found on the platform's website (https://www.uclouvain.be/asm.html).

Representative References

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- PIETER L.H., VERLOOY P.L.H., ROBEYNS K., VAN MEERVELT L., LEBEDEV O.I., VAN TENDELOO G., MARTENS J.A., KIRSCHHOCK C.E.A. Synthesis and characterization of the new cyclosilicate hydrate (hexamethylene-imine)$_4$·[$Si_8O_{16}(OH)_4$]·12H_2O. Microporous and Mesoporous Materials 130: 14-20. **2010**.
- KESSNER U., KASCHTA J., STADLER F.J., LE DUFF C.S., DROOGHAAG X., MÜNSTEDT H. Thermorheological behavior of various short- and long-chain branched polyethylenes and their correlations with the molecular structure. Macromolecules 43(17): 7341-7350. **2010**.

Funding

- Université catholique de Louvain (UCL)

Main Equipment

- XRD: Rigaku Rotating anode (Mo radiation) equipped with Xenocs mirrors, MAR345 image plate and Oxford Cryostream (80K to 400K)
- Liquid-state NMR:
  - 4 Bruker NMR spectrometers
  - 2 spectrometers operating at 300MHz for ^{1}H
  - 2 spectrometers operating at 500MHz for ^{1}H
- MS: Q-Exactive HRMS spectrometer with HPLC system

Products and Services

- Tailored analyses involving X-Ray Diffraction (XRD), liquid-state NMR spectroscopy and high-resolution Mass Spectrometry (MS)
- Hands-on analyses and consulting (NMR, XRD and MS)

Keywords

Molecule
Analysis
Structure
Single crystal diffraction
Liquid-state NMR spectroscopy
Mass spectrometry

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Ab initio study of materials at the nanoscale

SENIOR SCIENTISTS

- Jean-Christophe CHARLIER
- Xavier GONZE
- Gian-Marco RIGNANESE

Research Field and Subjects

Firstprinciples - or *ab initio* - simulations allow the prediction, based on quantum mechanics and electromagnetism, of many properties of materials, from their knowledge at the atomic scale. Predictable properties range from optical spectra and electric transport to mechanical, dielectric or magnetic responses, etc. Based on advanced formalisms, such as density-functional theory (DFT) and many-body perturbation theory, sophisticated software applications are run on powerful parallel computers, enabling the exploration of various materials, *e.g.* oxides or graphene-based nanostructures, bulk or doped, their surfaces and interfaces.

As a first goal, we aim to gain an understanding of the electronic and optical properties of high-technology materials, such as materials for photovoltaics (*e.g.* CZTS), for light-emitting diodes (LED) or siliconbased technology (Metal/Oxide/Silicon in particular, and also new high-k dielectrics). Recently, new p-type transparent conducting oxides (TCOs) have been identified.

Another goal consists of understanding the quantum transport properties in organic molecules and graphene-based nanostructures using advanced digital techniques. Our simulations are based not only on the *ab initio*-description (DFT formalism within the Landauer-Buttiker approach and beyond), but also on tight-binding models enriched by first-principles calculations (using the Kubo-Greenwood approach).

The development of first-principles software application ABINIT (http://www.abinit.org), used worldwide, is also a major part of our activities.

Representative References

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- LHERBIER A., BOTELLO-MENDEZ A.R., CHARLIER J.-C. Electronic and transport properties of unbalanced sublattice N-doping in grapheme. Nano Letters 13(4): 1446-1450. **2013**.
- DA PIEVE F., DI MATTEO S., RANGEL T., GIANTOMASSI M., LAMOEN D., RIGNANESE G.-M., GONZE X. Origin of magnetism and quasiparticle properties in Cr-doped TiO_2. Physical Review Letters 110(13): 136402. **2013**.
- LV R., LI Q., BOTELLO-MENDEZ A.R., HAYASHI T., WANG B., BERKDEMIR A., HAO Q., ELIAS A.L., CRUZ-SILVA R., GUTIERREZ H.R., KIM Y.A., MURAMATSU H., ZHU J., ENDO M., TERRONES H., CHARLIER J-C., PAN M., TERRONES M. Nitrogen-doped graphene: beyond single substitution and enhanced molecular sensing. Scientific Reports 2: 586. **2012**.
- STANKOVSKI M., ANTONIUS G., WAROQUIERS D., MIGLIO A., DIXIT H., SANKARAN K., GIANTOMASSI M., GONZE X., COTE M., RIGNANESE G.-M. The G^0W^0 band gap of ZnO: effects of plasmon-pole models. Physical Review B 84(24): 241201. **2011**.
- LHERBIER A., DUBOIS S.M.-M., DECLERCK X., ROCHE S., NIQUET Y.M., CHARLIER J.-C. Two-dimensional Graphene with structural defects: elastic mean free path, minimum conductivity and Anderson transition. Physical Review Letters 106: 046803-046806. **2011**.
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Awards

- Agathon De Potter Prize in Physics 2009-2011, awarded by the Royal Academy of Belgium (J.-C. Charlier)
- Election of X. Gonze as member of the Royal Academy of Belgium, Classe des Sciences, on March 5, 2011
- Quinquennal prize of the F.R.S.-FNRS in applied exact sciences 2006-2010 (X. Gonze)

Funding

- Fonds de la Recherche Scientifique (F.R.S-FNRS)
- Fonds de la Recherche Scientifique (F.R.S-FNRS): Fonds pour la Formation à la Recherche dans l'Industrie et l'Agriculture (FRIA)
- European Commission: 7th Framework Programme
- European Commission: 7th Framework Programme, ICT FET Flagship
- Fédération Wallonie-Bruxelles: Action de Recherche Concertée (ARC)
- BASF research contract
- Massachusetts Institute of Technology (MIT)-Université catholique de Louvain (UCL) Seed Fund
- Service Public de Wallonie (SPW), Plan Marshall

Partnership

- European Theoretical Spectroscopy Facility (ETSF): network of more than 50 research teams, mainly within Europe
- Université de Liège (Belgium)
- Commissariat à l'Energie Atomique (CEA) Bruyères-le-Châtel, Grenoble (France)
- Université de Montréal (Canada)
- Universidad San Sebastián (Chile)
- Massachusetts Institute of Technology (MIT) (USA)
- Lawrence Berkeley National Laboratory (LBNL) (USA)
- Wallonia Network for Nanotechnologies (NanoWal) (Belgium)

Main Equipment

- ETSF Test farm: more than 20 computers, with different OS, compilers, libraries

Products and Services

- The ETSF offers its expertise to researchers, industry, and students in the form of collaborative projects, free scientific software and training. Proposals to benefit from these services can be submitted at any moment, and are evaluated twice a year by an external scientific panel

Keywords

Ab initio computation
Carbon nanotubes
Graphene
Condensed matter theory
Electronic properties
Numerical simulations
Transparent conducting oxides
Optical properties

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Graphene: from synthesis to the tailoring

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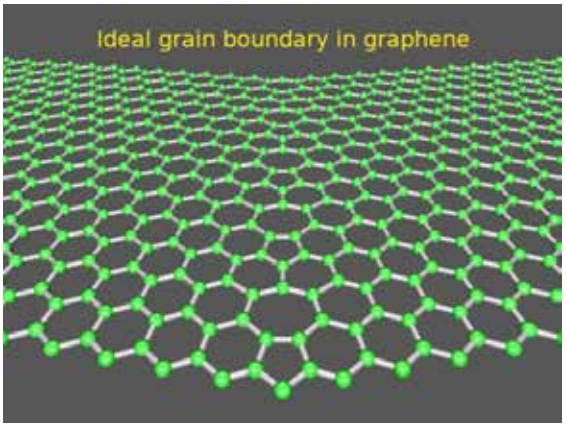
- Philippe LAMBIN
- Jean-Jacques PIREAUX
- Robert SPORKEN

Research Field and Subjects



Graphene is a truly two-dimensional crystal composed of carbon whose atoms form a chickenwire-like network with strong covalent bonds. Graphite is a piling of an almost infinite number of graphene sheets bound together by weak van der Waals forces. Many interesting properties of graphene put this material at the foreground of present day nanoscience. Graphene is mechanically hard, extremely flexible, chemically inert, impermeable to any atom and molecule and optically transparent. It is a zero-gap semiconductor easily made conducting by electrostatic charging, the charge carriers having then a remarkable mobility, and it has excellent thermal conductivity. The electronic properties of graphene are highly dependent on its environment, which makes it a good candidate for sensing. Initially isolated from graphite by skilful exfoliation, then obtained by annealing of carbon terminated (0001) face of SiC, graphene is most commonly produced today by thermal decomposition of hydrocarbon molecules at the surface of a metal held at high temperature. Copper foil, leading to high areas of monolayer graphene, is widely used for this.

The research conducted at the *Université de Namur* covers all these fields, including synthesis and characterisation (diffraction, spectroscopy, microscopy) of samples produced by the techniques mentioned above. Chemical doping of graphene grown on SiC is achieved by plasma treatment. Functionalisation of graphene is conducted with the aim of endowing it with specific reactivity. In parallel to these experimental efforts, electronic and vibrational properties of graphene are identified digitally to learn how they are influenced by mechanical strain or by a particular lattice defect, edge, grain boundary, impurity or adsorbed molecule, and could therefore be tailored for specific applications. Plasmons and electromagnetic properties of graphene nanostructures are also under investigation in the quest for new optical and shielding effects.

Representative References

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- FELTEN A., FLAVEL B.S., HIRTZ M., BRITNEL L., ECKMAN A., LOUETTE P., PIREAUX J.-J., KRUPKE R., CASIRAGHI C. Single- and double-sided chemical functionalization of bilayer graphene. Small 9(4): 631-639. **2013**.
- MARK G.I., VANCSO P., LAMBIN P., HWANG C., BIRO L.P. Forming electronic waveguides from graphene grain boundaries. Journal of Nanophotonics 6(1): 061718 1-6. **2012**.
- LAMBIN P., AMARA H., DUCASTELLE F., HENRARD L. Long-range interactions between substitutional nitrogen dopants in graphene: Electronic properties calculations. Physical Review B 86(4): 045448 1-10. **2012**.
- JOUCKEN F., TISON Y., LAGOUTE J., DUMONT J., CABOSART D., ZHENG B., REPAIN. V., CHACON C., GIRARD Y., BOTELLO-MENDEZ A.R., ROUSSET S., SPORKEN R., CHARLIER J.C., HENRARD L. Localized state and charge transfer in nitrogen-doped graphene. Physical Review B 85(16): 161408(R) 1-5. **2012**.

Award

- Prix Charles Courtoy UNamur 2011 (A. Felten)

Funding

- Université de Namur (UNamur)
- Fonds de la Recherche Scientifique (F.R.S.-FNRS)
- European Commission: Research Executive Agency (REA)
- Vietnam International Education Development (VIED)

Partnership

- Wallonia Network for Nanotechnologies (NanoWal) (Belgium)
- FNRS Contact Group «Nanostructure» (Belgium)
- Centre National de la Recherche Scientifique - Groupement de Recherche International (CNRS-GDRI) «Graphene and Nanotubes»

Main Equipment

- CVD reactors
- Chambers for plasma treatment
- Auger electron spectroscopy (AES)
- X-ray photoemission spectroscopy (XPS)
- Scanning transmission electron microscope (STEM)
- Scanning tunneling microscope (STM) and Atomic force microscope (AFM)
- Interuniversity Scientific Computing Facilities - Plateforme Technologique de Calcul Intensif (ISCF -PTCI)

Products and Services

- Good knowledge of the field and of the literature
- Synthesis - doping - functionalisation - characterisation tools
- Modeling means for the interpretation of measurements

Keywords

Carbon
Chemical vapour deposition
Mechanical properties
Raman spectroscopy
Electronic properties
Plasmons
Nanotechnology

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Graphene: quantum transport and electro-mechanical properties

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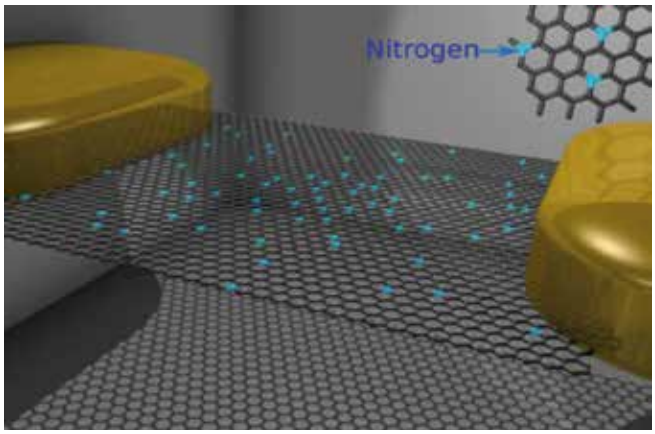
- Jean-Pierre RASKIN

Research Field and Subjects



Recent years have witnessed many breakthroughs in research on "Graphene" (the first two-dimensional atomic crystal) as well as a significant advances in the mass production of 2D materials. This one-atom-thick hexagonal network of carbon uniquely combines extreme mechanical strength, exceptionally high electronic and thermal conductivity, impermeability to gases, transparency to light and many other attractive properties, all of which make it highly suitable for numerous applications.

The present research group mainly focuses on the deep understanding of quantum transport and electro-mechanical properties in graphene using first-principles simulations and unique experimental capabilities developed at UCL. Based on a longstanding collaboration in the joint team of Pr J.-P. Raskin and Pr T. Pardoen, a strong expertise in the development of the nanolab-on-chip approach based on nanofabrication has been achieved, allowing generation and measurement controlled mechanical stress in graphene. Scanning tunnelling microscopy (STM) and scanning gate microscopy (SGM), both operating down to cryogenic temperatures and developed in the group of Pr B. Hackens, have already demonstrated their ability to uncover, decrypt and manipulate complex charge transport mechanisms inside graphene-based nano-devices. Finally, the *ab initio*-modelling at UCL, which has a worldwide reputation within the European Theoretical Spectroscopy Facility (ETSF), favours scientific collaborations around the world, with a specific expertise on graphene-based nanostructures.

Graphene is a unique crystal in the sense that it combines many superior properties, from mechanical to electronic. This suggests that its full power will only be realised in novel applications designed specifically with this 2D material in mind, rather than when it is used to replace other materials in existing applications (*i.e.* new technologies such as printable and flexible electronics, flexible solar cells, supercapacitors, etc.).

Representative References

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▸ SORIANO D., LECONTE N., ORDEJON P., CHARLIER J.C., PALACIOS J.-J., ROCHE S. Magnetoresistance and magnetic ordering fingerprints in hydrogenated grapheme. Physical Review Letters 107: 016602-016605. **2011**.

Awards

▸ Marcel de Merre Prize in Nanotechnology 2010, UCL (J.-P. Raskin)
▸ Alcan Prize 2011, the French Academy of Sciences (T. Pardoen)
▸ Agathon De Poetter Prize in Physics 2009-2011, the Royal Academy of Belgium (J.-C. Charlier)

Funding

▸ European Commission: 7th Framework Programme, ICT FET Flagship
▸ Fédération Wallonie-Bruxelles: Action de Recherche Concertée (ARC)
▸ Fonds de la Recherche Scientifique (F.R.S-FNRS)
▸ Massachusetts Institute of Technology (MIT)-Université catholique de Louvain (UCL) Seed Fund

Partnership

▸ European Theoretical Spectroscopy Facility (ETSF): network of more than 50 research teams, mainly within Europe
▸ Université catholique de Louvain (UCL), Research Center in Micro and Nanoscopic Materials and Electronic Devices (CeRMiN) (Belgium)
▸ Wallonia Network for Nano-technologies (NanoWal) (Belgium)

Main Equipment

▸ *ABINIT code*: modeling package whose main program allows to find properties of systems made of electrons and nuclei (periodic solids and nano-systems), on the basis of quantum mechanics and electromagnetism (first-principles calculations within density-functional theory–DFT). Atomic geometries are optimised according to the forces and stresses, molecular dynamics simulations can be performed and vibrational or dielectric properties can be also addressed. Excited states (optical properties) can be computed within the Time-Dependent Density Functional Theory (for molecules), or within Many-Body Perturbation Theory (GW approximation). Intensive scientific calculations are mainly performed on massively parallel computers at UCL.

▸ Graphene oven installed in Winfab (clean room facilities of UCL) for the CVD graphene deposition and a Raman spectrometer installed in Welcome (electrical characterisation platform at UCL) for the produced graphene analysis. Equipments for graphene device processing (lithography, etching, etc.) are also available in the Winfab facilities.
▸ Two scanning probe microscopes operating down to ultralow temperature (20mK) and high magnetic field (17T), allowing to combine electrical transport on nanodevices with local (nanometer-scale) microscopy and spectroscopy.

Products and Services

▸ Expertise offer to researchers, industry, and students in the form of collaborative projects, free scientific software and training

Keywords

Graphene
Carbon-based nanostructures
Electromechanical properties
Quantum transport
First principles calculations - *ab initio* modelling
Raman spectroscopy
Scanning tunnelling microscopy (STM)
Scanning gate microscopy (SGM)

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http://www.abinit.org
http://www.uclouvain.be/winfab
http://www.uclouvain.be/welcome

Bio-inspired photonic materials

SENIOR SCIENTISTS

- Jean Pol VIGNERON†
- Serge BERTHIER
- Olivier DEPARIS

Research Field and Subjects

A *Photuris* firefly, from Central America, flashes light from an abdominal lantern by way of bioluminescent chemical reactions. As a condensed-matter source, this lantern meets the same difficulties in extracting the light into the air. The study of the lantern's structure is the inspiration for the design of a light-extracting layer which can improve LED devices.

The objective of this research is the design and optimisation of photonic structures, *i.e.* inhomogeneous media that control the propagation of light. The starting point of these studies is always the analysis of processes that occur in nature and, in particular, in living organisms - animal or vegetal. Occasionally, mineral structures are examined, as numerous fibrous rocks have attracted considerable practical interest in the range of applications that are envisioned. The analysis of natural structures is a reverse engineering process, by which samples collected through different means are measured to produce information on their morphology and their optical properties and are understood through digital simulations. By "understanding", we mean that the observed optical properties are proven to originate from the observed geometry, given the known values of the refractive indexes. Such an objective requires a multidisciplinary approach, where some knowledge of biology, skills in optical and electron microscopy, knowledge of optical and radiometric measurements and computation capabilities are all of equal importance.

An important part of the research concerns the colouring effects of one-, two- and three-dimensional photonic crystal films. Weevils and longhorns, bird feathers, beetles and spiders, marine ctenophores, ants and bees, etc. are examples of photonic structures providing coloration. Other physical properties such as anisotropic friction coefficients, superhydrophobicity, anti-reflection and improved absorption, have been identified in these biological organisms, delivering starting points for engineering designs.

For examples: the light-extraction improvement from LED devices was guided by a detailed study of the lantern of some fireflies; anti-reflecting and self-cleaning surfaces for solar thermal or photovoltaic sensors were studied starting from the surface of cicadas' wings; a super-diffuser film was designed based on the structure of the shell of a sea-snail and hygrochrome materials were developed, taking the cuticle of some colour-changing beetles as blueprints.

Representative References

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Patent

- Functional multilayer system. WO 2013/164255 (A1), 2013 (Application number WO 2013/EP58668, 2013; Priority number EP 2012/0166155, 2012).

Funding

- Service Public de Wallonie (SPW), Programme Greenomat
- Fédération Wallonie-Bruxelles: Action de Recherche Concertée (ARC)

Partnership

- Université catholique de Louvain (UCL) (Belgium)
- Université de Liège (ULg) (Belgium)
- Université de Mons (UMONS) (Belgium)
- Materia Nova (Belgium)
- European Synchrotron Radiation Facility (ESRF) (France)
- Smithsonian Tropical Research Institute (Republic of Panama)

Main Equipment

- Interuniversity Scientific Computing Facilities (ISCF), Université de Namur
- Optical measurements (spectrophotometry)
- Light diffusion measurements
- Scanning electron microscopy
- Optical microscopy and fluoroscopy
- Entomology facilities

Products and Services

- Consultance on photonics

Keywords

Photonic crystals
Bragg mirrors
Nanostructures
Photonics

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Conformal coating of ultrathin inorganic layers for applications in electronics, energetics and photonics

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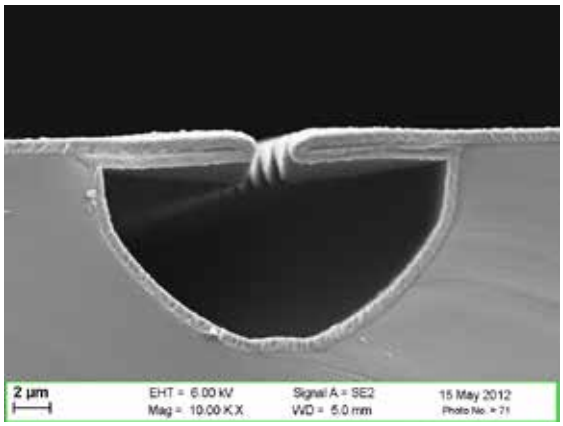
Research Field and Subjects



With the current trend in extreme miniaturisation, the precise control of thin-film coatings provides a cost-effective means to improve the performance of electronic and optical components considerably. Over the years, specific expertise has been achieved within the Wallonia Infrastructure NanoFABrication (WINFAB) clean-room environment regarding deposition processes controlled at the atomic level and the development of *in situ* diagnostic probes to monitor in different real-time deposition processes.

The clean-room, for example, is equipped with a remote-plasma atomic layer deposition tool (ALD, Fiji F200 from Ultratech Cambridge NanoTech Inc.) and a DC/RF reactive sputtering tool (AJA International Inc.). These tools allow the coating of highly conformal ultrathin (a few hundred nanometers or less), atomically controlled and low temperature (down to room temperature) layers of various materials on different types of substrates. Thanks to the low temperature, the tools can accommodate ceramic, metal, glass or polymer planar substrates up to 8" in diameter. The tools offer great flexibility in terms of materials, *i.e.*, for the thin-film deposition of pure or doped metal oxides (ITO, ZnO, Al_2O_3, TiO_2, HfO_2, La_2O_3, etc.), metal nitrides (AlN and TiN) and pure metals (Al, Ti, Pt, Pd, etc.). These deposition techniques are adapted for multilayer coatings, and material compounds can be obtained from the pure metals by the reactive sputtering technique. Thanks to the high conformality, regular thick layers can perfectly coat three-dimensional and porous structures.

Thin-film coatings have applications in electronics, energetics and photonics. To date, the expertise has mostly been applied to obtain functional smart materials for micro- and nano-electromechanical systems (MEMS/NEMS) such as gas sensors, as dielectrics for new generation transistors (single electron transistors and memories), as conductive or passivation layers for silicon photovoltaics cells, as bio-inspired photonics structures applied to anti-counterfeiting, etc.

One of the *in situ* measurement techniques consists in following the curvature of the substrate (typically Si or glass) at very high resolution (10 km^{-1} at a rate of 0.1 s) and is installed on the reactive sputtering tool. Such *in situ* curvature measurements do not only provide useful nano- and micro-mechanical information on the growing coatings, but also on the kinetics and mechanistic details of the growth process itself.

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Patent

- Device, method and system for improved uptake, storage and release of hydrogen. WO 2012/156332 (A1), 2012 (Application number WO 2012/EP58832, 2012; Priority numbers WO 2011/EP58164, 2011 – WO 2011/EP60823, 2011).

Award

- Best Graduate Student Paper Award, 7th International Conference on Diffusion in Solids and Liquids - Special Session on Hydrogen-related Kinetics in Materials, 2011 (R. Delmelle, O. de Liedekerke de Pailhe, S. Michotte, J. Proost)

Funding

- Fonds de la Recherche Scientifique (F.R.S.-FNRS)
- Fédération Wallonie-Bruxelles: Fonds Spécial de Recherche (FSR) UCL, Action de Recherche Concertée (ARC) Académie Universitaire Louvain
- European Regional Development Fund (ERDF)
- Service Public de Wallonie (SPW)
- Wallonie-Bruxelles International (WBI)

Partnership

- AGC Flat Glass Europe
- Université de Sherbrooke, Institut interdisciplinaire d'innovation technologique - 3IT (Canada)
- Institut des Nanotechnologies de Lyon (INL) (France)

Main Equipment

- Remote-plasma atomic layer deposition tool with *in situ* ellipsometry
- Reactive DC/RF magnetron sputtering equipment with *in situ* internal stress monitoring capability

Keywords

In situ stress monitoring
Reactive sputtering
Remote-plasma atomic layer deposition
Photovoltaics
Photonics
Single electron memories
Single electron transistor
Anti-counterfeiting

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Nonlinear optical properties of molecules, materials and interfacial systems

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- Yves CAUDANO
- Aurélie PLAQUET
- Vincent LIEGEOIS
- Benoît CHAMPAGNE

Research Field and Subjects

Nonlinear optical (NLO) spectroscopies are used to measure the vibrational, electronic and optical properties of molecular films at interfaces. In particular, we explore the interface of (bio-)organic thin films adsorbed on solids with vibrational and electronic NLO spectroscopies (*i.e.* sum frequency generation – SFG, and second harmonic generation – SHG). The systems investigated include self-assembled monolayers on metal or semiconducting materials, model lipid membranes interacting with biological species or with nanomaterials, or liquid crystal films with strong NLO activities. An important area is the coupling of NLO processes with localised plasmon resonances (LSPR) in nanostructured substrates. These systems are platforms for sensing devices, biological models for nanotoxicity studies, as well as materials for optically active devices. Research activities in fluids mechanics are also carried out, with the challenge to provide a new understanding of the dynamical phenomena at the very boundary between fluids and solids, down to the molecular level.

Methodological approaches to predict and interpret the NLO properties of molecules, polymers, surfaces, and molecular crystals have been developed and scientific codes are implemented on the High Performance Computing (HPC) architectures of the *"Consortium des Equipements de Calcul Intensif"* (CECI). They allow:

- Unravelling of structure/NLO property relationships;
- Design of molecules and supramolecules with targeted NLO responses, for instance with regard to their application as sensors;
- Simulation and interpretation of the spectroscopic electronic and vibrational NLO responses of functionalised surfaces;
- Prediction of the bulk responses from the molecular properties.

Recent applications have dealt with molecular switches, chiral compounds, metal-organic frameworks and multiradicalar systems including nanographenes.

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Patent

- Method for enhancing a sum frequency generation signal. WO 2013/160376 (A1), 2013 (Application number WO 2013/EP58546, 2013; Priority number EP 2012/0165496, 2012).

Funding

- Fonds de la Recherche Scientifique (F.S.R.-FNRS)
- Belgian Science Policy (BELSPO): Interuniversity Attraction Poles (IAP)
- Fédération Wallonie-Bruxelles: Fonds Spécial de Recherche (FSR)
- Service Public de Wallonie (SPW)

Partnership

- Université catholique de Louvain (UCL) (Belgium)
- Katholieke Universiteit Leuven (KULeuven) (Belgium)
- Université de Liège (ULg) (Belgium)
- Université de Bordeaux (France)
- Université de Lyon 1 (France)
- Université de Paris-Sud 11 (France)
- Max-Planck-Institut für Polymerforschung (MPIP) (Germany)
- Jagiellonian University in Krakow (Poland)
- Bulgarian Academy of Sciences (Bulgaria)
- Sherbrooke University (Canada)
- Osaka University (Japan)

Main Equipment

- Picosecond SFG spectrometer
- Femtosecond SHG spectrometer
- HPC center of «*Plateforme Technologique de Calcul Intensif*» (PTCI) (UNamur) and CECI

Products and Services

- SFG and SHG spectrometers to measure the NLO vibrational and electronic responses of surfaces and interfaces
- Scientific codes to evaluate the NLO responses

Keywords

Thin films
Nanoparticles
Nanostructures
NLO properties
First principles calculations, second and sum frequency generations

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Bio and soft electronics for sensors and implantable electrodes

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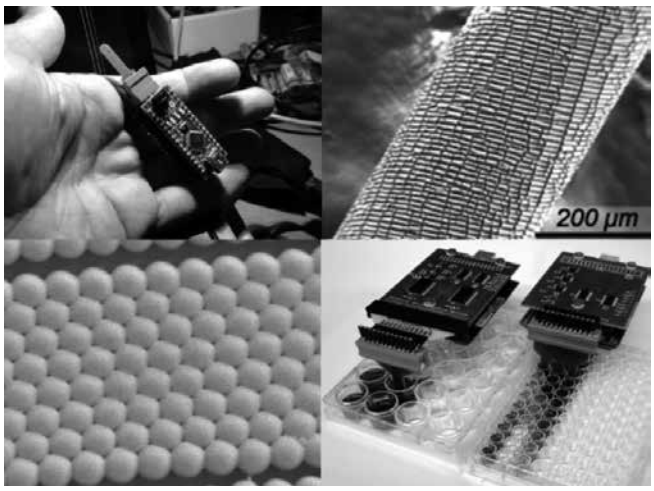
- Patrick BERTRAND
- Arnaud DELCORTE
- Claude POLEUNIS

Research Field and Subjects



The development of new synthetic approaches and methods for hierarchical assembly is becoming essential especially in structuring materials down to micro- and nanometer scale for real applications. In this context, our main expertise concerns the development of new micro- and nano-devices for bio-sensing and/or neuro-stimulation. In addition to micro- and nanofabrication, a large part of our research is devoted to the development of new electrochemical methods adapted to these new devices. As a consequence of these two approaches, the laboratory has gained considerable experience in the fabrication of real working devices such as portable USB biosensors that take advantage of cutting-edge technologies (*e.g.* the use of electro-conductive polymer materials).

Our research includes many other related fields such as surface characterisation, thin organic films and supra-molecular assemblies, biomaterials and hybrid materials, plasma treatments, chemical grafting, conducting polymer film growth, electrospinning, electrochemistry, thin (organic/metallic) layer adsorption, soft lithography, breath figure imprinting, micro-fluidics, etc.

The group has a long history of collaboration with partners from university and industry research centres.

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Patents

- Stretchable conductor and method for producing the same. US 2010/089616 (A1), 2010 (Application number US 2007/0594400, 2007; Priority number WO 2007/EP53159, 2007).
- Smart sensor system using an electroactive polymer. WO 2011082837 (A1), 2011 (Application number WO 2010/EP57753, 2010; Priority number EP 2010/0150280, 2010).

Funding

- Service Public de Wallonie (SPW): Direction Générale Opérationnelle de l'Economie, de l'Emploi et de la Recherche (DGO6), Programme First Spin-off, Plan Marshall

Partnership

- Ecole Polytechnique Fédérale de Lausanne (EPFL), Laboratoire de Production Microtechnique (LPM) (Switzerland)
- Université de Liège (ULg), Centre d'Ingénierie des Protéines (CIP) (Belgium)
- Centre d'Etude et de Recherche sur les Macromolécules (CERM) (Belgium)
- Consiglio Nazionale delle Ricerche (CNR), Istituto per lo Studio delle Macromolecole (ISMAC) (Italy)
- Gymetrics SA (Switzerland)
- Aquatic Science SA (Belgium)

Main Equipment

- Chemistry Laboratory for materials synthesis and functionalisation
- Electronic Laboratory for PCB manufacturing and electrical characterisation
- Process Laboratory for microfluidics fabrication and plasma treatment facilities
- Home-made USB transportable potentiostats and disposable electrodes for easy and fast biosensing kit development

Products and Services

- Home-made USB transportable potentiostats and disposable electrodes for easy and fast biosensing kit development

Keywords

Biosensors
Implantable electrodes
Polydimethylsiloxane (PDMS)
Enzymes
Electrochemistry
Microfluidics
Electro-conductive polymers

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Magnetic nanowired materials for RF electronics

SENIOR SCIENTISTS

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Research Field and Subjects

In order to reduce the size of microwave devices, ferromagnetic nanowires embedded into porous templates are an interesting alternative to ferrite-based materials. The work of the groups of I. Huynen and L. Piraux at UCL is at the leading edge in this field. Over the last decade, they have successfully prepared a variety of ferromagnetic nanowired substrates and demonstrated the ability to build planar reciprocal and non-reciprocal devices for very high frequencies, as currently required for wireless communication and automotive systems. Indeed, such templates were recently used to design various microwave devices, such as circulators, isolators and phase shifters.

The main advantage of ferromagnetic nanowired substrates is that they present a zero-field microwave absorption frequency thanks to the very high aspect ratio of the nanowires. The zero-field microwave absorption frequency can be easily tuned over a wide range of frequencies by the appropriate choice of materials. In contrast, in order to operate conventional ferrite devices need to be biased by a magnetic field provided by a permanent magnet, which constitutes a negative point in view of volume reduction. Other advantages of such materials compared to traditional ferrites are a higher operation frequency, a higher saturation magnetisation, and improved temperature stability. These advantages make such planar materials highly competitive as compared to traditional ferrite-based hybrid solutions used for microwave signal processing, especially for on-board aeronautic and space applications requiring weight and size reduction together with stability in severe temperature and vibration conditions.

Prototypes of (nonreciprocal) microwave circulators and phase shifters have already been successfully demonstrated on ferromagnetic substrates. Additionally, the presence of ferromagnetic material is responsible for an increase in the permeability at low frequency and the tuneability in frequency when an external DC magnetic field is applied. Tuneability performance of integrated inductances and the quality factor predicted by simulations were successfully validated by experiment. Tuneability is also of great interest for filters and novel compact devices using the metamaterial concept, combining negative permittivity and permeability of substrates.

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Funding

- European Commission: 7th Framework Programme, Marie Curie Actions
- Service Public de Wallonie (SPW)
- Fondation Louvain
- Fonds de la Recherche Scientifique (F.R.S.-FNRS)
- Fonds de la Recherche Scientifique (F.R.S.-FNRS): Fonds pour la Formation à la Recherche dans l'Industrie et l'Agriculture (FRIA)
- Industrial fundings

Partnership

- THALES Alenia Space
- THALES Systèmes Aéroportés
- Universidad Autónoma de San Luis Potosí (Mexico)

Main Equipment

- High vacuum coating systems (sputtering and e-beam)
- Electrochemical set-up
- High Resolution Scanning Electron Microscopy & EDX probe
- Network analyser combined with cryogenics and magnetic field facilities
- WELCOME Measuring Facility

Products and Services

- Fabrication and characterisation tools for magnetic nanowired materials
- Thin metal film deposition vacuum coating
- Multiparametric electrical measurement of RF devices (under various humidity, temperature, mechanical stress conditions)

Keywords

Nanotechnology
Nanowired substrates
High frequency characterisation
Thin film vacuum deposition
Electrodeposition
Microwaves devices

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Multi-hierarchical composites for controlling the propagation of electromagnetic waves

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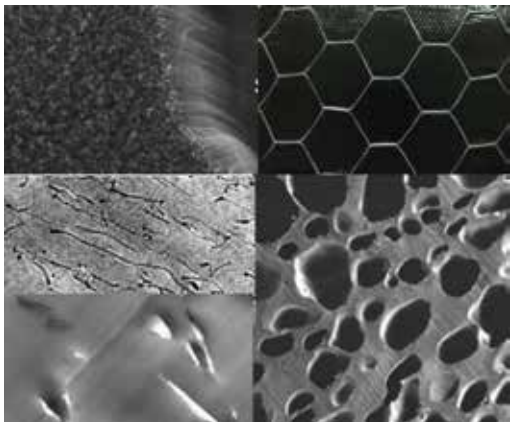
- Sophie HERMANS
- Isabelle HUYNEN
- Thomas PARDOEN

Research Field and Subjects



The research aims to demonstrate the potential of the intelligent hierarchisation of nanoscaled inclusions in composite materials for controlling the electromagnetic (EM) propagation at wavelengths ranging from millimetres up to a ten of centimetres. Synergies are first envisioned at the nanoscale between carbonaceous and metallic nanoparticles in order to generate unusual combinations of material EM properties, *i.e.* the permittivity and magnetic permeability. To this end, nanotubes or graphene are decorated by magnetic nanoparticles. These are prepared by deposition/precipitation, or by strategies involving covalent grafting of molecular precursors. In particular, molecular mixed-metal clusters might be used to obtain bimetallic nanoparticles from a single-source precursor. In order to create anchors on carbonaceous surfaces, functionalisation strategies involving mainly radical chemistry or pi-pi stacking are implemented.

Next, cutting-edge chemical functionalisation and polymer processing techniques combined with state-of-the-art nano- and microscale characterisation techniques will provide unprecedented control over the hierarchical organisation of inclusions in a polymer hosting matrix, from the nano- to the millimetre scale, together with extensive possibilities of conforming and moulding.

Finally, synergy between nano- and millimetre-scaled reinforcing structures is exploited to further enhance EM performance and confer multifunctionality to a single material, for instance combined absorption of EM waves and mechanical shocks/impacts, or joint electrical and thermal insulation/absorption.

This approach enables the design of compact multifunctional EM metamaterials displaying electromagnetic properties not found in nature and of prime interest to the field of smart electronics and wireless communications. Cloaking invisibility of objects, sub-wavelength size reduction and absorbers of electromagnetic interferences are some of the developments in progress over various frequency ranges, going from optics to GHz.

Representative References

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Patents

- Hybrid material for electromagnetic absorption. WO 2012/032117 (A1), 2012 (Application number WO 2011/EP65554, 2011; Priority number EP 2010/0175887, 2010).
- Process for preparing electromagnetic interference shielding materials. WO 2012/028734 (A1), 2012 (Application number WO 2011EP65237, 2011; Priority number EP 2010/0175224, 2010).

- Polymer composite material structures comprising carbon based inductive loads. WO 2008/068042 (A2), 2008 (Application number WO 2007/EP10786, 2007; Priority numbers EP 2006/0025002, 2006 – EP 2007/0010440, 2007).

Funding

- European Commission: 7th Framework Programme
- European Science Foundation (ESF): European Cooperation in Science and Technology (COST)
- Fonds de la Recherche Scientifique (F.R.S-FNRS)
- Fonds de la Recherche Scientifique (F.R.S-FNRS): Fonds pour la Formation à la Recherche dans l'Industrie et l'Agriculture (FRIA)
- Fédération Wallonie-Bruxelles: Action de Recherche Concertée (ARC) Académie Universitaire Louvain
- Agentschap voor Innovatie door Wetenschap en Technologie (IWT)
- Fonds Européen de Développement Régional (FEDER)
- Belgian Science Policy Office (BELSPO), Interuniversity Attraction Poles (IAP)
- Service Public de Wallonie (SPW), Direction Générale Opérationnelle de l'Economie, de l'Emploi et de la Recherche (DGO6), Plan Marshall

Partnership

The complementarity between principal investigators favors fruitful collaborations in the frame of numerous projects funded at the regional and federal level and ensures its international competitiveness.

- Belgian collaborations (non-exhaustive list):

Academic: Cenaero, Certech, Cetic, Sirris, Materia Nova, University of Liège (CERM group), UMONS, UNamur

Industrial: Nanocyl, AGC-Flat Glass, Alstom, Solvay, Thalès Alenia Space Etca, SEE Electronics

- International collaborations: Institut de Physique et Chimie des Matériaux de Strasbourg (IPCMS), Benoît Pichon (France)
- *Academic*: partners of collaborative projects

Main Equipment

- Inorganic chemistry lab:
  - Gloveboxes, autoclaves, Schlenk vacuum lines for syntheses under inert atmosphere;
  - Infrared and Raman spectroscopy with *in situ* cell;
  - Thermogravimetric analyses;
  - Textural characterisations.
- BSMA:
  - Polymer processing;
  - Thermal and thermomechanical analysis;
  - Rheology coupled with dielectric spectroscopy;
  - Microscopy.
- SUCH technological platform: Electronic and ionic spectroscopies for the chemical characterisation of surfaces and thin films
- WELCOME technological platform:

Broadband electromagnetic characterisation of materials in free-space, anechoic, and circuit/system configuration for smart electronics and communications, using:

  - LCR meters for dielectric spectroscopy;
  - Vector network analysers;
  - Near field measurements setups;
  - Anechoic chamber;
  - Climatic rooms.
- iMMC:

Nano-, micro- and macro-mechanical testing, involving nanoindentation, adhesion, fatigue, impact and fracture testing in controlled temperature and environment.

Multiscale finite element simulations of representative volume elements.

Products and Services

- WELCOME answers measurements needs in the electronics and communication fields of industry in Belgium and abroad, in the frame of (sub)contracts and consultancy.

With some regulation policy, trainings for R&D engineers from industry are also possible.

Keywords

Nanoparticles
Graphene
Nanotubes
Hybrid
Multifunctionality
Foam

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Technology platform: Wallonia ELectronics and COmmunications MEasurements (WELCOME) A facility making a bridge from molecules to signals

SENIOR SCIENTIST

- Isabelle HUYNEN

Research Field and Subjects

The Wallonia ELectronics and COmmunications MEasurements (WELCOME) facility is a state-of-the-art technological platform providing multi-disciplinary tools in the field of electrical and electro-magnetic characterisation. It is located in the Institute of Information and Communication Technologies, Electronics and Applied Mathematics (ICTEAM). For more than 10 years, expertise in the field of nanosciences and materials has been jointly developed with the Institute of Condensed Matter and Nanosciences (ICMN) and the Institute of Mechanics, Materials and Civil Engineering (iMMC) of UCL.

Available tools and techniques in WELCOME result from various research foci including micro- and nanotechnology (materials and devices), silicon-on-insulator technology, radiofrequency (RF) and microwave circuits, digital systems and VLSI architectures, micro/nano electromechanical systems (MEMS/NEMS), cryptography, ultra-low power wireless (bio)sensors, molecular electronics and wireless communications between sensors. WELCOME covers in a broad and unified approach the electrical and electromagnetic characterisation of nanomaterials and sensors under various stimuli, ranging from their physical behaviour to system architectures and ultra-wideband communications protocols between them.

The platform offers support to research in nanoscience and materials such as:

- Nanoelectronics, through the characterisation of active nanodevices over a broad frequency range (from DC to 110GHz), including physical (*e.g.* interface or thin layer properties) and mechanical (adhesion, stress, etc.) characterisation;
- Nanospintronics, through the characterisation of ferromagnetic nanowires at microwave frequencies for the design of novel RF devices;
- Electromechanical characterisation of MEMS/NEMS sensors for RF and biomedical applications, at wafer-scale as well as packaged circuits levels;
- Carbon-based composite materials (carbon nanotubes and graphene) for smart RF electronics;
- Molecular electronics and scanning tunnelling microscope imaging of nanostructures;
- Characterisation (DC, RF) from cryogenic temperatures (4 K) to high temperatures (300°C).

Representative References

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Patents

- Hybrid material for electromagnetic absorption. WO 2012/032117 (A1), 2012.

- Process for preparing electromagnetic interference shielding materials. WO 2012/028734 (A1), 2012.
- Network architecture for wirelessly interfacing sensors at ultra low power. WO 2009/092771 (A1), 2009.
- Double-gate floating-body memory device. WO 2009/087125 (A1), 2009.
- Ultra-low-power circuit. WO 2008/132210, 2008.
- Imposing and determining stress in sub-micron samples. WO 2008/098993 (A2), 2008.
- Polymer composite material structures comprising carbon based conductive loads. WO 2008/068042 (A2), 2008.
- Internal stress actuated micro- and nanomachines for testing physical properties of micro and nano-sized material samples. WO 2007/093018 (A2), 2007.
- Method of manufacturing a multilayer semiconductor structure with reduced ohmic losses. WO 2005/031842 (A2), 2005.
- Process for manufacturing a multilayer structure made from semiconducting materials. WO 2005/031853 (A1), 2005.
- Method and device for high sensitivity detection of the presence of DNA and other probes. WO 2004/001403 (A1), 2004.

Funding

- European Commission: 6th and 7th Framework Programmes
- European Science Foundation (ESF), European Cooperation in Science and Technology (COST)
- Fonds de la Recherche Scientifique (F.R.S.-FNRS)
- Fonds de la Recherche Scientifique (F.R.S.-FNRS): Fonds pour la Formation à la Recherche dans l'Industrie et l'Agriculture (FRIA)
- Fédération Wallonie-Bruxelles: Action de Recherche Concertée (ARC)
- Agentschap voor Innovatie door Wetenschap en Technologie (IWT)
- Fonds Européen de Développement Régional (FEDER)
- Belgian Science Policy Office (BELSPO), Interuniversity Attraction Poles (IAP)
- Service Public de Wallonie (SPW), Direction Générale Opérationnelle de l'Economie, de l'Emploi et de la Recherche (DGO6), Plan Marshall

Partnership

The WELCOME facility is complementary in many aspects to resources and skills available in nearby research centers active in similar fields. This complementarily favors fruitful collaborations in the frame of numerous projects funded at the regional and federal level and ensures its international competitiveness.

- Belgian collaborations (non-exhaustive list):

Academic: UCL-WINFAB, Cenaero, Certech, Cetic, Sirris, Materia Nova, ULg-Microsys, IMEC, KULeuven, Multitel, UGent, ULg, ULB/VUB, UMONS, UNamur,…

Industrial: Icoms, Melexis, nSilition, Nanocyl, CISSOID, IMEC, AGC-Flat Glass, Solvay, On Semi Belgium, Arcelor Mittal, Thalès Alenia Space Etca, Thalès Communications Belgium

- International collaborations:

Academic: Partners of collaborative projects listed above: CEA-LETI (France), MINATEC (France), IEMN (France), University of Cambridge (United Kingdom), University of Warwick (United Kingdom),…

Industrial: SOITEC (France), ST-Microelectronics (France), Thalès TRT (France), EADS (France, Germany), IBM (USA), RFMD (USA), OKI (Japan),…

Main Equipment

- Various coaxial setups, on-wafer probe stations and Vector Network Analyzers configurations to achieve a multi-port (up to 4 accesses) and multi-parametric characterisation of (nano)materials, electron devices and sensors (IV, CV, temperature-microwave, electro-mechanical, and magneto-electrical sweeps, …), in small-signal and nonlinear regime, from DC to 110 GHz, in the temperature range 4K-500K
- Low current probes, logical analysers, analog waveform and digital pattern generators, digital oscilloscopes, vector signal generators with I/Q or digital modulation for analog/digital circuits and systems-in-package (smart cards, RFIDs, FPGAs) interfacing with (nano)sensors
- Scanning tunneling microscope
- Climatic chambers for measurements in controlled humidity and temperature environment)
- Polytech vibrometer for interferometric measurements of Micro- and Nano-electromechanical Systems
- Anechoic chamber for electromagnetic testing of nanocomposite materials and sensors
- RF hardware for wireless and ultra-wideband communications between (nano)sensors
- Micro-Raman spectroscopy

Products and Services

WELCOME answers needs of industry in Belgium and abroad, in the frame of (sub)contracts and consultancy. With some regulation policy, trainings for R&D engineers from industry are also possible.

- DC and RF characterisation of active and passive (nano) devices,sensors, and circuits under various conditions (voltage and current bias, temperature, humidity, mechanical stress, gas flow, radiation, laser illumination,…)
- 3-D dynamic characterisation of MEMS and MOEMS microstructures (in and out-of-plane vibrations, surface topography under pressure stimuli)
- Electrical characterisation of various bulk and composite materials (liquid, solid, film, powder), from DC to 75 GHz
- EMI shielding and radiation of materials, antennas and sensors in anechoic chamber

Keywords

Spintronics
Composites
Thin films
Molecular electronics
MEMS/NEMS
Nano(bio) sensors
Multiparametric and broadband electrical characterisation

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Technology platform: Wallonia Infrastructure Nano FABrication (WINFAB) Micro- and nano-fabrication

SENIOR SCIENTISTS

- Romain DELAMARE
- Benoît HACKENS
- Mathieu VANDEN BULCKE

Research Field and Subjects

The Wallonia Infrastructure Nano Fabrication (WINFAB) is the technological platform of UCL for micro- and nano-fabrication. It is an inter-institute platform within the Sciences and Technology Sector. Currently, the main research activities in WINFAB are focused on the following topics: SOI (Silicon-on-Insulator)-CMOS integrated circuit processing, Micro(Nano) Electromechanical Systems (MEMS/NEMS), nanoelectronics, organic electronics, photovoltaics, solar hydrogen, micro fuel cells, bioactive surfaces and biosensors.

Besides the processing of various types of materials (polymers, semiconductors, dielectrics,.etc.), activities are also carried out in the field of materials development (thin films, metamaterials, composites, two-dimensional crystal synthesis, etc.) and characterisation.

The cleanroom infrastructure of about 1000 m^2, distributed over two levels and divided into 13 thematic areas, houses a lot of high technology equipment.

The process line is based on 3-inches silicon wafers. Some of the equipment can accommodate smaller and larger wafer sizes, as well as different substrate materials. The panel of available equipment allows the users to experiment with standard and non-standard micro- and nano-fabrication process steps, applied on various substrates, but also to work on more applications-oriented processing aimed at modifying or adding functional properties to materials.

Representative References

- CAMPOS-DELGADO J., ALGARA-SILLER G., SANTOS C.N., KAISER U., RASKIN J.-P. Twisted bi-layer graphene: microscopic rainbows. Small 9(19): 3247-3251. **2013**.
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Funding

- European Commission: Network of Excellence (NoE)
- European Commission: 7th Framework Programme
- European Consortium for Accreditation (ECA)
- Belgian Science Policy Office (BELSPO), Interuniversity Attraction Poles (IAP)
- Fonds de la Recherche Scientifique (F.R.S.-FNRS)
- Service Public de Wallonie (SPW), Programmes d'Excellence, Plan Marshall
- Fonds Européen de Développement Régional (FEDER)

Partnership

- As technological platform, WINFAB opens its infrastructure to external users from university or industry
- Technical training for teachers, workers, students, and unemployed through Technifutur (www.technifutur.be/formations/)

Main Equipment

- Cleanroom environment
- Characterisation (microscopy, ellipsometry, profilometry,…)
- Wet benches (substrate cleaning, wet etch,…) and dry etching (RIE, DRIE)
- UV lithography (spin coating, exposure, development)
- E-beam nanolithography
- Nano-imprint lithography
- Furnaces (Oxidation, LP CVD nitride and PolySi, anneal,…)
- Thin film (reactive sputtering, evaporation, Atomic Layer Deposition, PE CVD nitride and oxide,…)
- Ion implanter
- Glove boxes
- MEMS release (CPD)
- Pre- / Post processing (wafer grinding, CMP,…)
- Laser micro machining
- Packaging (dicing, wire bonding,…)

Products and Services

- Cleanroom work environment
- Realisation of individual or set of process steps (cleaning, etching, lithography, characterisation,…)
- MEMS, Sensors and SOI CMOS Processing
- Education and training

Keywords

Cleanroom
Micro- and nanoelectronics
CMOS
SOI
MEMS
Sensors
Organic electronics
Photovoltaics

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Keywords Index

Supported catalysts	**D1, D3**
Supported oxides	**D2**
Surface characterisation	**D6**
Surface chemistry	**D1**
Surface modification	**D6**
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* Technology platform

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Van Velthem Pascal	**B1, D7***
Vanden Bulcke Mathieu	**E11***
Vigneron Jean-Pol †	**C2, E4**
Vincent Stéphane	**A3**
Wouters Johan	**A5**
Yunus Sami	**D6, E7**

* Technology platform



The Académie universitaire Louvain (AL) is a university consortium composed of the following three academic institutions: UCL, UNamur and Saint-Louis. The Research Administration Departments of the Académie universitaire Louvain aim at promoting and facilitating academic collaboration with outside partners (companies, research centres and other public bodies).

The mission of the Research Administration Departments is multiple:

- to initiate and stimulate the relations between research laboratories, companies and/or public bodies;
- to facilitate knowledge transfer and contribute to the third mission of the university « service to society »;
- to contribute to the regional economic development through cooperation with local actors;
- to promote the development of innovative products and services and the setting-up of spin-offs;
- to guarantee the best management of intellectual property;
- to inform the researchers (dissemination of the information on available funding sources) and to advise the researchers (legal and financial expertise);
- to assist the researchers at several stages of their research project (identification of the available funding sources, application for the funding best matching their needs, contract negotiation, appropriate management of the obtained funds during the project lifetime);
- to ensure the dissemination and monitoring of research contracts inside the academy.

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