GRAPHENE-CA

Coordination Action for Graphene-Driven Revolutions in ICT and Beyond

Coordination and support action

WP3 Defining the Research Agenda

Deliverable 3.2 “Research agenda for the GRAPHENE flagship”

Main Author(s):

Jari Kinaret, Vladimir Falko, Andrea Ferrari, Jani Kivioja, Tomas Löfwander, Daniel Neumaier, Konstantin Novoselov, Vincenzo Palermo, Stephan Roche

Nature of deliverable: R = Report
Dissemination level: PU = Public
Due date of deliverable: M12
Actual submission date: M12

Project funded by the European Commission under grant agreement n°284558

LIST OF CONTRIBUTORS

Partner	Acronym	Laboratory Name	Name of the contact
1(coordinator)	CUT	Chalmers tekniska hoegskola	Jari Kinaret
2	UNIMAN	The University of Manchester	Andre Geim
3	UNILAN	Lancaster University	Vladimir Falko
4	UCAM _DENG	The Chancellor, Masters, and Scholars of the University of Cambridge	Andrea Ferrari
5	AMO	Gesellschaft fuer angewandte Mikro- und Optoelektronik mit beschraenkter Haftung AMO GmbH	Daniel Neumaier
6	ICN	Catalan institute of nanotechnology	Stephan Roche
7	CNR	Consiglio nazionale delle ricerche	Vincenzo Palermo
8	NOKIA	Nokia OYJ	Jani Kivioja
9	ESF	Fondation Européenne de la Science	Ana Helman

TABLE OF CONTENTS

Deliverable Summary

In this Deliverable, we present the scientific vision of the GRAPHENE flagship and the matching of our vision with the flagship concept. We outline the research agenda in the 10-year perspective, and lay out the work plan for the ramp-up phase. The activities for the first 30-month period have been organized into 11 interconnected scientific and technological work packages: (1) Materials, (2) Health & environment, (3) Fundamental science, (4) High-speed electronics, (5) Optoelectronics, (6) Spintronics, (7) Sensors, (8) Flexible electronics, (9) Energy applications, (10) Nano-composites, and (11) Production. The WPs are strongly interlinked, both in terms of facilities and methods used in the studies, researchers involved, and practical outcomes. Graphene research is still undergoing explosive growth. As a result, we expect a number of unpredicted discoveries in the field, and will in the flagship continuously monitor and assess scientific developments that may open new technological opportunities.

1. Scientific vision, unifying goal, and main objectives of the flagship, in comparison with the current state-of-the-art

Our mission is to take graphene and related layered materials from a state of raw potential to a point where they can revolutionize multiple industries - from flexible, wearable and transparent electronics, to high performance computing and spintronics. This will bring a new dimension to future technology-a faster, thinner, stronger, flexible, and broadband revolution. Our program will put Europe firmly at the heart of the process, with a manifold return on the investment of 1 billion Euros, both in terms of technological innovation and economic exploitation.

The flagship will bring together a focused, interdisciplinary European research community that aims at a radical technology shift in information and communication technology that exploits the unique properties of graphene and related two-dimensional materials. Graphene research is an example of an emerging *translational nanotechnology* where discoveries in academic laboratories are rapidly transferred to applications. The concept translational nanotechnology is typically associated with biomedicine where it is a well-established link between basic research and clinical studies, but the principle can be applied to ICT as well: the most striking example thus far is giant magnetoresistance that moved from an academic discovery to a dominant information storage technology in a matter of a few years. Similarly, *graphene and related two-dimensional materials have the potential to make a profound impact in ICT in the short and long term:* Integrating graphene components with silicon-based electronics, and gradually replacing silicon in some applications, allows not only substantial performance improvements but, more importantly, it enables completely new applications. The flagship will serve as a sustainable incubator of new branches of ICTs applications, rooted on European scientific excellence and interdisciplinarity, merging physics with chemistry and engineering communities.

Graphene is the material with most superlatives: it is the best conductor of heat we know, the thinnest material, it conducts electricity much better than silicon, is 100-300 times stronger than steel, has unique optical properties, it is impermeable already as a monolayer, and it only relies on one of the most abundant materials on Earth, carbon. Either separately or in various combinations, these superlative properties can be exploited in many areas of research; new possibilities are being recognized all the time as the science of graphene and other two-dimensional materials progresses. The flagship will serve as a vessel to bring these fruits of European research breakthroughs to the benefit of Europeans as new energy-efficient and environmentally friendly products, new jobs, and increased economic growth.

During the Coordination Action pilot phase, the European graphene community has been mobilized to prepare for the large scale flagship program GRAPHENE that will integrate the research chain from fundamental science, through developing new engineering concepts, to commercializable applications. Due to the unique structure of graphene, many of the possibilities it offers are still poorly understood, and their analysis requires highly sophisticated methods; to quote the Nobel Laureate Frank Wilczek from the Nobel Symposium on graphene held in Stockholm in May 2010, « *graphene is probably the only system where ideas from quantum field theory can lead to patentable innovations* ». As a preparatory step towards the flagship, the pilot Coordination Action has produced a scientific and technological roadmap targeting and fostering innovative industrial applications including, *e.g.*, graphene electronics, spintronics, photonics, and plasmonics. In the GRAPHENE Flagship, we will develop graphene electronics that can sustain ICT devices and technologies evolution beyond the limits achievable with silicon. By exploiting the unique electrical and optical properties of graphene and related two-dimensional materials, we will develop novel systems for information processing and communication. These will include charge based electronic devices with ultra-high speed of operation as well as non-charge based devices (for instance spintronic devices) with novel functionalities. We will advance methods to produce cheap graphene materials, which combine structural functions with embedded electronics, in an environmentally sustainable manner. The GRAPHENE flagship will extend beyond mainstream ICT to incorporate novel sensor applications and composite materials that take advantage of the extraordinary chemical, biological and mechanical properties of graphene.

Beyond the core ICT activities, the flagship will reach out to several related areas. Graphene's good electrical conductivity and large surface area per unit mass make it an exciting material for energy storage applications such as advanced batteries and supercapacitors, which will have a large impact on portable electronics and other key technological areas such as electric cars: the prospect of rapidly chargeable lightweight batteries would give environmentally friendly transportation a major push and advance the large scale implementation of electric cars as a key component in urban and suburban transportation in Europe. Strong and lightweight composites would allow us to build new cars, airplanes and other structures with less material and energy, and contribute positively to a more sustainable Europe.

Carbon has been the driving force behind several technological revolutions: in the 19th century, energy production by burning carbon was integral to the industrial revolution; in the 20th century, carbon-based plastics revolutionized the manufacturing industry; and in the 21st century, graphitic carbon is a likely key component in a third technological revolution, this time centered around information and communication technologies. This project is the first, coordinated European initiative to prepare for this predicted development, and assure that European industries will have a major role area. A successful implementation of this vision in a Flagship will have a profound impact in the lives of Europeans through the competitiveness of European industries and the creation of new jobs in the European Union.

Since the start of the graphene revolution in 2004, numerous application concepts based on graphene have been demonstrated. In just a few years, high-frequency graphene transistors have reached performance that rivals that of the best semiconductor devices that have over sixty years research effort behind them; graphene electronics is still very much at its infancy and, extrapolating from recent progress, we expect graphene devices to break the 1 THz barrier in a matter of a few years.[1]

In optoelectronics, the first graphene-based touch screen was recently demonstrated in a collaboration between SKK University and Samsung in Korea.[2] The touch screen application is expected to be one of the first to be commercialized, partly because the materials choice is quite limited: the screens must exhibit both electrical and optical functionalities, and very few

---

[1] "The Nobel Prize in Physics 2010". Nobelprize.org. 4 July 2011 http://nobelprize.org/nobel_prizes/physics/laureates/2010/. Geim, A. K. and Novoselov, K. S. The rise of graphene. *Nature Mater.* **6**, 183 (2007). Bonaccorso, F., Sun, Z., Hasan, T. and Ferrari, A. C. Graphene photonics and optoelectronics. *Nature Photon.* **4**, 611 (2010). Mueller *et al.* Graphene photodetectors for high-speed optical communications. *Nature Photon.* **4**,297 (2010). Wu,YQ *et al*. High-frequency, scaled graphene transistors on diamond-like carbon Nature **472,** 74 (2011).

[2] Bae, S. *et al.* Roll-to-roll production of 30-inch graphene films for transparent electrodes. *Nature Nanotech.* **4**, 574 (2010).

materials conduct both electricity (like metals) and light (like window glass). Presently, touch screens rely on limited resources such as indium that is only available from a few sources, predominantly in China, while graphene is essentially an unlimited resource – carbon is one of the most common elements on Earth.

Graphene has been used to produce tunable lasers by exploiting the material's unusual electronic structure that guarantees a wide tunability range.[3] Graphene's properties also imply that the percentage of light absorbed decreases when the incoming light intensity increases, which can be exploited to fabricate very fast pulsed lasers that have great potential in optical communication.

However, despite the great progress in graphene science and technology during the past six years, the field is still very young and many challenges remain. Some of the challenges are fundamental: due to the unique structure of graphene, many of the possibilities it offers are still poorly understood, and their analysis requires highly sophisticated methods. Among these fundamental challenges are a detailed understanding of the properties of finite graphene structures and graphene multilayers and the role that edges play in them, and magnetic properties of graphene and the possibility to use spin rather than charge as the information carrier.

Many of the major experimental challenges have to do with materials supply. There are several methods to produce graphene – on the laboratory scale, mechanical exfoliation ("Scotch tape method") works well but is difficult to scale-up, while the techniques of chemical exfoliation, chemical vapor deposition and sublimation of silicon carbide are in principle all upscalable and have different strengths and weaknesses. Reliable and sufficiently large scale production of graphene with consistent quality is a crucial necessary step before graphene science can evolve into a graphene technology. More recently, a new class of graphene-like two-dimensional materials such as boron nitride and different metal chalcogenides has rapidly emerged as interesting supplements to the new materials palette for electronics.[4] At this point, these materials have not been thoroughly explored, and their full potential has not yet been assessed.

Different application areas have their own research challenges: for instance, the main hurdle that presently blocks the development of digital graphene electronics is the absence of an energy gap, which makes it very difficult to turn transistors off and limit leakage currents, while in analog electronics the related challenge is sufficient power amplification so that several graphene transistors can be connected in series.[5] These engineering challenges spawn new innovative solutions such as the BiSFET that relies on the gapless nature of graphene to create a new type of a transistor, and regard ambipolarity as a new asset rather than a deficiency,[6] or the TFET, where the bandgap-tunable nature of bilayer graphene can allow efficient switching with no need to manufacture ribbons.[7]

---

[3] Sun, Z. *et al.* Graphene mode-locked ultrafast laser. *ACS Nano* **4,** 803 (2010).

[4] Coleman, J. N. et al. Two-dimensional nanosheets produced by liquid exfoliation of layered materials. Science **331**, 568 (2011).

[5] Lin, YM, et al. Wafer-Scale Graphene Integrated Circuit. Science **332,** 1294 (2011).

[6] Banerjee, Sanjay K. et al. Bilayer PseudoSpin Field-Effect Transistor (BiSFET): A Proposed New Logic Device IEEE Electron Device Letters, **30**, 158 (2009)

[7] G. Fiori**,** G. Iannaccone, On the possibility of tunable-gap bilayer graphene FET. IEEE Electron Device Letters, **30**, 261 264, (2009)

2. Matching of Flagship proposal with Flagship concept

Graphene has the potential to make a profound impact in ICT in the short and long term: Integrating graphene components with silicon-based electronics, and gradually replacing silicon in some applications, allows not only substantial performance improvements but, more importantly, enables completely new applications. As an added value, graphene has great potential beyond ICT in energy and environment related applications such as batteries, supercapacitors, and lightweight composites.

In this respect, graphene represents a disruptive technology shift, and, as such, faces great uncertainties and challenges. While we are convinced that graphene will make a revolutionary impact in ICT, it is much harder to pinpoint which applications will emerge first. In consumer electronics the volumes are so large – for instance, 44 mobile telephones are sold worldwide every second – that a reliable supply of materials and components is an absolute requirement. A systems manufacturer will not develop a new technology unless it can be certain of the security of component supply, while the component producer depends similarly on the materials supply and on the demand from the systems manufacturer.

A strength of a concentrated effort, such as the flagship, is that *it can address all parts of the value chain* and catalyze the technology shift that no single player or branch would dare to undertake on their own. The branching of the value chain – usage of the same materials or components in different applications – is another strength of such an approach. It allows the actors to pursue simultaneously the low-hanging fruits, the first applications, and the larger strategic goal.

The community interested in this young and fast growing research field is at present fragmented, divided into national efforts, several EU projects and networks. This leads to disconnected and in some cases duplication of efforts. For instance, all projects must at present include material production. Short term projects (typically 3 years) carries with them the risk that knowledge gets lost as the consortiums are disintegrated and partners continue in new directions in new projects. The flagship is a more long-term project, which allows a coordinated effort that will eliminate fragmentation, avoid duplication of work, and create synergies between different areas: the flagship concept is the most economic option as illustrated in Figure 1.

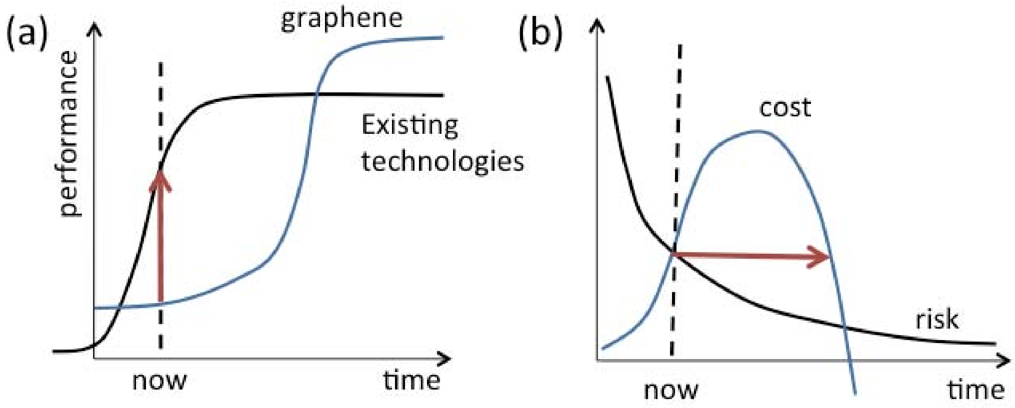


***Figure 1**: The graphene flagship will integrate the entire value chain, thereby minimizing the financial and technological risks associated with launching a new technology. The coordinated European level effort will overcome the gap between the laboratory and the market place in a way that no single country or company can do.*

3. Description of methodology, strategic research roadmap with milestones, and work plan for ramp-up phase

The scientific and technological roadmap for graphene and related two-dimensional materials has been developed during the pilot phase. It is based on inputs from the international academic and industrial research community collected through workshops, conferences, and reading of supplied and open-source documents. The vast amount of information has been collected in a 200 page document. This document forms the base for the Flagship work-plan for the ramp-up phase and beyond.

In constructing the roadmap and the work-plan it became increasingly clear that graphene has a realistic chance to become the next disruptive technology. For a disruptive technology, a roadmap will necessarily take a quite different form compared with a roadmap for an evolutionary technology, as for instance the ITRS for semiconductors. In order to become disruptive, a technology needs to offer not incremental, but dramatic, order of magnitude, improvements over the existing state of the art. The more universal the technology, the better chances it has for broad base success. Consider plastics, they are being used everywhere, from automotive industry and health to packaging and electronics. In terms of its properties graphene certainly has the potential. Many of its characteristics are unique and superior to those of other materials. More importantly, graphene offers an extensive combination of the “super”-properties. So, it is really a question of how many applications graphene can be used for and how pervasive it can become. Are the properties of graphene indeed so unique that they will overshadow inconveniences of the switching to a new technology, a process usually accompanied by large R&D and capital investments?

One of the reasons for the incredibly fast progress of graphene research is the multitude of very special properties observed in this 2D crystal: it possesses a number of characteristics which are unique or superior to those of other materials. Graphene holds the leading position in many parameters, including mechanical stiffness, strength and elasticity, electrical and thermal conductivity, it is optically active, chemically inert, impermeable to gases, and so on… These properties allow graphene to earn its place in current technologies as a replacement for other materials in existing applications. For instance, in principle, graphene with its high electrical and thermal conductivities could be used for interconnects in integrated circuits in place of copper and its high mechanical stiffness would allow its use for ultrastrong composite materials.

However, what makes this 2D crystal really special and what gives it a chance to become disruptive is that all these properties are combined in one material. The combination of transparency-conductivity- elasticity will find uses in flexible electronics; high mobility-ultimate thinness in efficient transistors for RF applications, transparency-impermeability-conductivity for transparent protective coatings and barrier films. The list of such combinations is endless and grows day by day. The most important combinations are probably those which have not been explored yet, as they would lead to new, revolutionary applications, which were unthinkable prior to the isolation of graphene in 2004.

Currently several record high characteristics have been achieved with graphene, with some reaching theoretically predicted limits: room temperature electron mobility of 2.5×10^5 $cm^2/V\cdot s$ (theoretical limit ~2×10^5 $cm^2/V\cdot s$); a Young modulus of 1TPa and intrinsic strength of 130GPa (very close to that obtained in theory); complete impermeability to any gases and so on. It has also been documented to have a record high thermal conductivity and can sustain extremely high densities of electric current (million times higher than copper).

Graphene’s many superior properties demonstrate that it may indeed be a miracle material. However, some of these characteristics have been achieved only for the highest quality samples, mechanically exfoliated graphene, and for graphene deposited on special substrates like hexagonal boron nitride. As yet, equivalent characteristics have not been observed on graphene prepared by other techniques, though these methods are improving day by day. The area will receive even greater attention from industry when it will be proven that mass-produced graphene can have the same outstanding performance as the best samples obtained in research laboratories.

Below, in Figures 2 and 3, we summarize the graphene roadmap. The illustrations intend to show how we can exploit the unique graphene material platform for a wide range of applications in ICT, energy, materials, health and beyond, as well as the currently expected timelines for realizing competitive components and taking them to market.

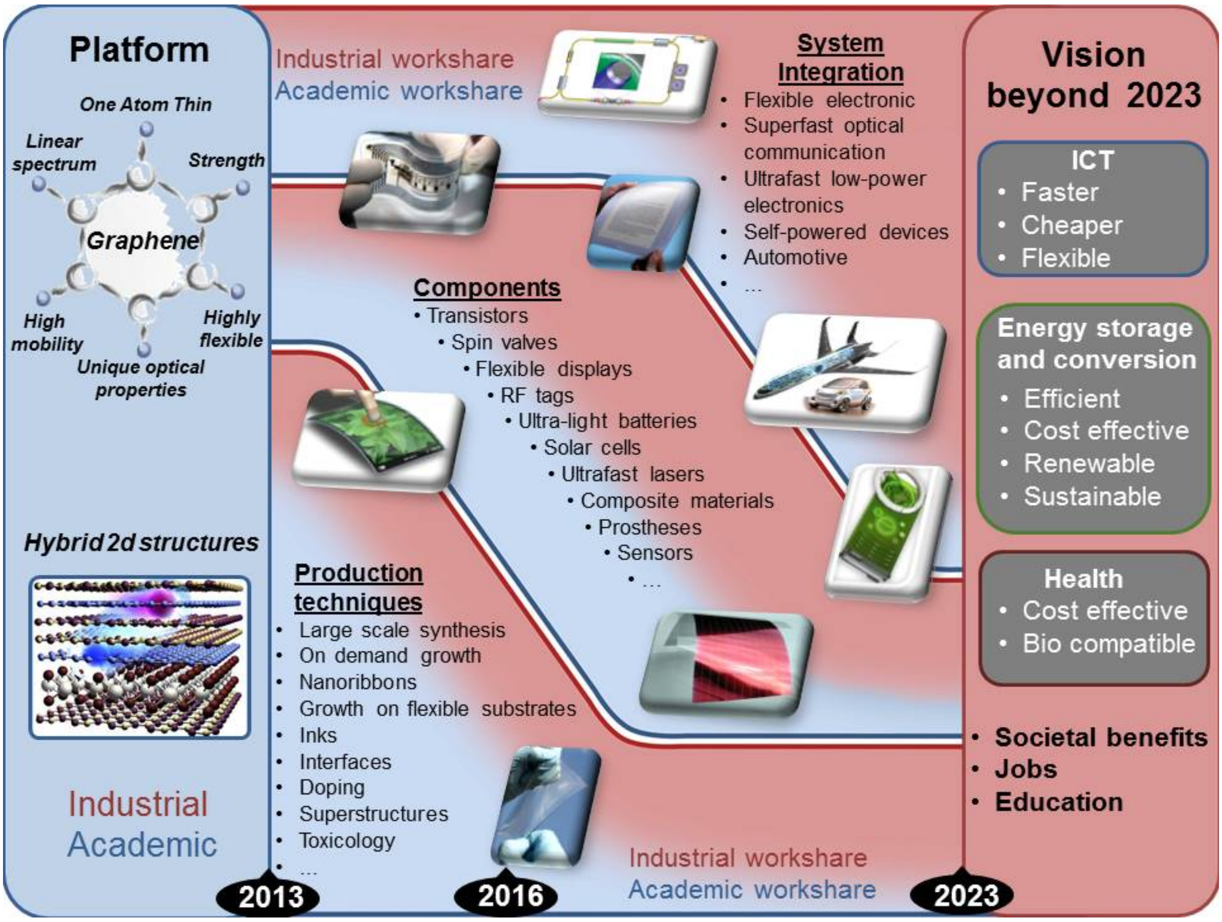


***Figure 2**: Illustration of the European graphene roadmap for the period of 2013-2023 and beyond for exploitation of the unique graphene material platform for a wide range of applications in ICT, energy, materials and beyond.*

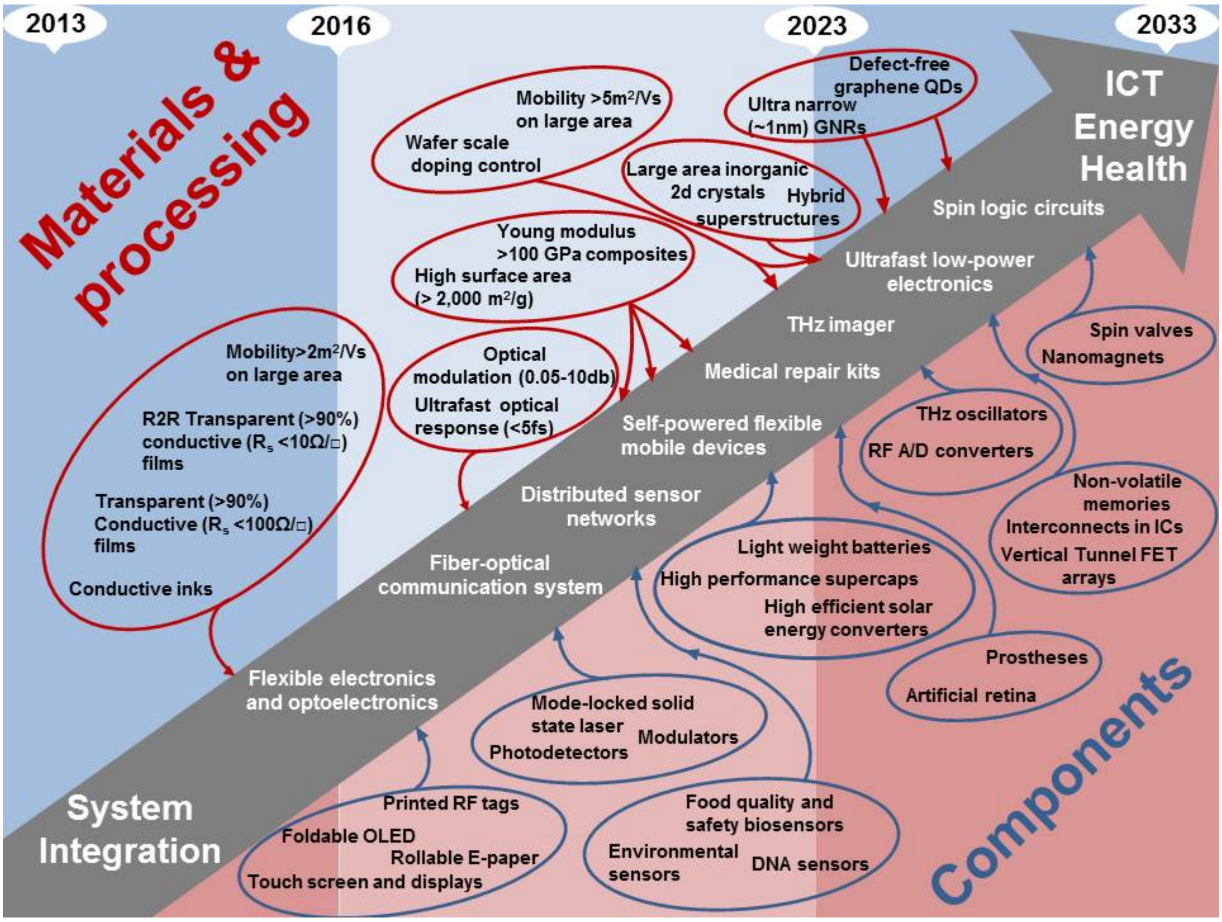


Figure 3*: Illustration of the European graphene roadmap for the period of 2013-2023 and beyond for the development of materials and processes needed for a wide range of components and applications, and the vision to bring these components to market.*

The **research agenda** for the Flagship is based upon the graphene scientific and technological roadmap outlined above. The research agenda has been defined in broad terms with long-term goals for the full 10-year period and in more detail in the form work plans for the first 30-month period, where the latter period coincides with the foreseen CP-CSA project in the 7th framework programme. The research has been divided into 11 scientific work packages. These can be grouped into topics of increasing levels of maturity with regards to closeness to industrial applications, see Figure 4 below. Naturally, for the first 30-month period of the flagship, industry will be more involved in the work packages covering more mature topics while academia will be involved in more fundamental studies. As time progresses, we foresee that several topics will mature and move from tier 1 into tier 2 and further into tier 3, with increasing industrial participation.

The WPs are strongly interlinked, both in terms of facilities and methods used in the studies, researchers involved and practical outcomes. Inter-WP coordination is a priority of the flagship, and will be addressed specifically in flagship organization and internal dissemination procedures.

Graphene research is still undergoing explosive growth. As a result, we expect a number of unpredicted discoveries in the field, and will in the flagship continuously monitor and assess scientific developments that may open new technological opportunities. We expect that these opportunities will lead to new work packages once the evolving fields have reached sufficient scope and maturity, and the necessary funds become available.

Below we lay out the research agenda for the eleven scientific and technological work packages. The WPs on dissemination and management are described in Chapters 3-4.

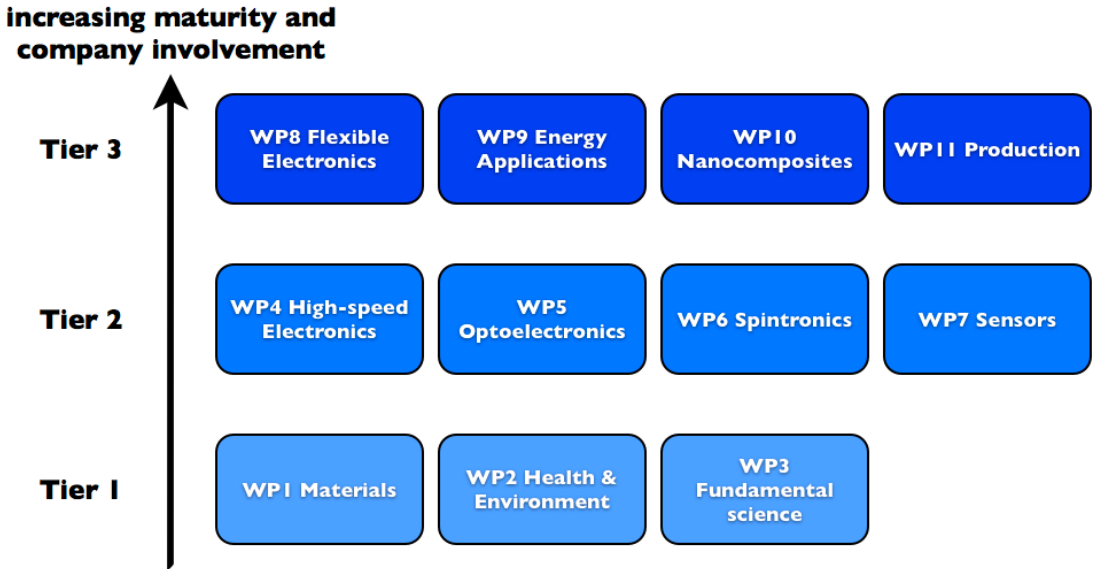


Figure 4: *The eleven scientific and technological work packages of the GRAPHENE flagship grouped according to increasing maturity and closeness to application. There are more partners from industry in the WPs covering more mature topics.*

3.1 WP1: Materials

The major challenges for the development of the technology for large-scale production of graphene-based products are access to large quantities of high-quality uniform graphene and the tailoring of graphene properties on demand.

The main focus of the Materials WP in a 10-year perspective is to achieve on-demand large-scale graphene structures and two-dimensional hybrid systems, with control of growth, pattern formation, functionalization and self-assembly without compromising the quality of the graphene layer.

In the first 30-month period, four basic targets are addressed within Materials WP:

1. Developing scalable synthesis protocols that enable the tuning of graphene electronic, structural and optical properties for different applications.
2. Enlarging the scope of graphene applications by adding new functionalities. This implies a complete strategy for covalent and non-covalent functionalization of graphene with molecules, clusters and nanocrystals.
3. Developing hybrid structures conformed by graphene and other 2D materials that can be the basis of new devices.
4. Systematic exploring other 2D materials, as there exist hundreds of layered materials that have not been exfoliated and that could exhibit, as graphene, extremely interesting properties that would be useful in a range of applications. In particular, metal transition chalcogenides and other metal transition layered materials will be explored

The combination of graphene with other materials in heterostructures as well as graphene functionalization will play a key role in validating graphene as a disruptive new nanotechnological platform for real-world devices. In the short term, we must meet the material specifications required by the applications targeted by other WPs and develop scalable strategies to build up few-layer-graphene heterostructures with improved functionalities.

Several methodologies will be exploited to develop efficient and scalable synthetic routes so as to tailor graphene properties:

- Growth of epitaxial graphene on SiC.
- CVD growth of graphene, multilayers and hybrids on metals, metal alloys and insulators in vacuum, atmospheric and high pressure as well as at high and low temperatures.
- MBE growth of graphene and hybrid heterostructures.
- Synthesis of graphene and its derivatives from molecular precursors. Graphene nano-ribbons.
- Large scale chemical and electrochemical exfoliation of graphene sheets using graphite as precursor.
- Functionalization and doping of graphene by chemical and physical routes.
- Chemical and electrochemical techniques to obtain new 2D-materials.
- Full characterization of the synthesized materials and hybrids by the most updated techniques.
- Theoretical and modeling support to the experimental groups.

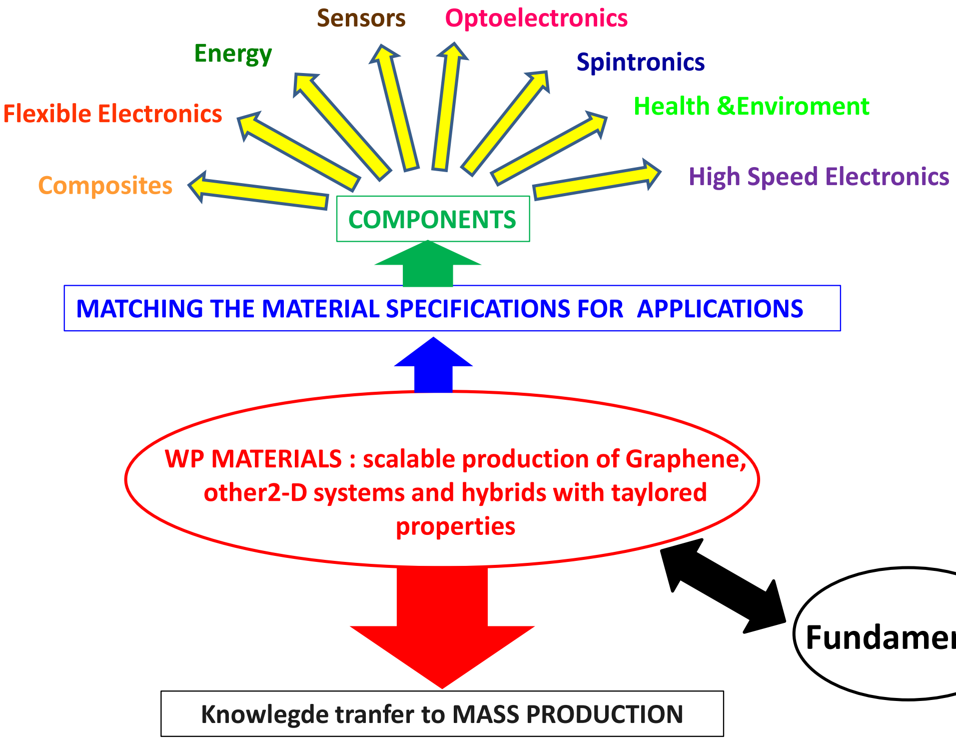


***Figure** 5: Interaction map that relates WP materials to the whole Flagship-Value-Chain.*

3.2 WP2: Health & Environment

Nanosafety research is an essential requirement that cannot be dissociated from the development of new nanotechnologies.[8,9,10,11] The graphene family nanomaterials (GFNs) and other 2D crystals and hybrids are envisioned as revolutionary products of nanotechnologies; however, their small size and their unique physico-chemical properties pose potential risks to the health of humans and the environment. Determining and resolving any safety and toxicity issues associated with these 2D structures will not only be beneficial to their integration into new materials for composites, nanoelectronics, etc. but also in case of their possible biomedical applications, which are currently being explored such as direct neuro-interfacing with cells and tissues.

A series of studies have been devoted to assess the *in vitro* and *in vivo* toxicity effects of graphene-based nanomaterials, while the same type of studies are lacking for the other 2D crystals. Some of the studies clearly showed no particular risks while others have evidenced that graphene might become a health hazard material. In the 10-year perspective, a careful analysis of the multiple graphene forms and of the other hybrids and their interactions with living systems will allow better understanding of the differences between the family members and eventually a correlation of their impact on health and environment with their physico-chemical characteristics. To date, there are no available studies which focus on the ecotoxicology and environmental impact of graphene and its family members. It is also imperative to develop and broaden our knowledge in this area in order to better identify the potential effects on the environment in the short and long term. With the development of mass-scale graphene production, the multiplication of their uses and arrival in the marketplace, it is essential to assess exposure in real conditions and fully understand the life-cycle of this material. Without this, any assessment of health risks due to occupational or environmental exposure will remain uncertain.

The activities of the first 30 month period will focus on a thorough explanation of the biological responses and the toxicity effects of GFNs by taking into consideration their physico-chemical properties. Indeed, the variability between the different samples is currently extremely high. The toxicity of graphene seems closely associated to its surface functionalization. In relation to surface characteristics, size is the second important parameter that needs to be carefully considered. In addition, other key factors can be associated to the toxicity of new nanomaterials. The generation of oxygen reactive species, the indirect toxicity because of nanomaterial adsorption of important biomolecules, and physical toxicity associated to the interaction with the lipids (and other molecules) constituting cell membranes, tissues and organs need to be carefully studied and analyzed. In addition, study of the cellular and tissue uptake as a function of GFN dimensions is necessary. Side dimensions of graphene might affect the population of receptors involved in possible energy-dependent penetration mechanisms (i.e. endocytosis/phagocytosis active mechanisms). If passive mechanisms are taking place, it is interesting to understand how the flat form of the material affects membrane organization (i.e. membrane disruption or simple sliding through the lipid bilayers). At the environmental level, the impact on certain number of aquatic species or microorganisms that can be generally affected once nanomaterials or other types of pollutants are released, will be assessed. New living organism models will be applied to investigate the water/sediment

---

[8] Kostarelos K, Bianco A, Prato M. Promises, facts and challenges for carbon nanotubes in imaging and therapeutics. Nat. Nanotechnol. 2009, 4, 627.

[9] Shvedova AA, Kagan VE, Fadeel B. Close encounters of the small kind: adverse effects of man-made materials interfacing with the nano-cosmos of biological systems. Annu. Rev. Pharmacol. Toxicol. 2010, 50, 63.

[10] Monopoli MP, Bombelli FB, Dawson KA. Nanobiotechnology: nanoparticle coronas take shape. Nat. Nanotechnol. 2011, 6, 11.

[11] Krug HF, Wick P. Nanotoxicology: an interdisciplinary challenge. Angew. Chem. Int. Ed. 2011, 50, 1260.

interface and terrestrial behavior of the different 2D nanoforms. All these studies will offer a safer design, production and manufacturing of 2D material platforms in order to minimize the risks for human health and environment.

Our specific and closely interconnected goals will be:

- to elucidate the mechanisms of how graphene forms and 2D crystals interact with cells at cellular and molecular level, with the assessment of the role of bio-corona of these nanomaterials
- to address the effects of graphene forms and 2D crystals on specific tissues such as the immune system, nervous system or placenta, and to determine biomarkers for possible pathogenic risks
- to identify any possible hazard of graphene forms and 2D crystals in relation to their physico-chemical properties with a special focus on the most important exposure routes (i.e. lung, skin)
- to understand the processes that control biostability and biodegradation of GFNs, key issues to open the route to neuro-interfacing devices
- to investigate the potential impact of the various 2D nanoforms on aquatic species (i.e. amphibians), terrestrial organisms and microorganisms
- to develop, at the national and international framework, a standardized and validated testing strategy for graphene forms and 2D crystals, to enable the regulation of these materials

To contribute to the development of a safe and sustainable nanotechnology based on graphene, 2D crystals and hybrids, it is fundamental to establish strong interactions with the other WPs. In particular, we plan to constantly exchange and collaborate with the partners of WP2 and WP6 dedicated to Materials and Nanocomposites, respectively. The development of graphene and 2D crystals, their complete characterization in terms of physico-chemical properties and their integration into new devices, envisaged in these two WPs, will be beneficial and fundamental to assess the impact on health and environment. In WP8 we will indeed test and explore the effects of these engineered nanomaterials in a systematic and comprehensive manner.

3.3 WP3: Fundamentals of graphene, new 2D materials, and hybrid structures

The purpose of this WP is to establish, *via* microscopic characterization and broad studies of kinetic processes, fundamental limits for a functionalizable use of graphene nanostructures, as well as to extend these limits by developing superstructures of graphene in conjunction with other two-dimensional (2D) crystals possessing a broad range of complementary properties.

In the 10-year perspective, to be able to exploit the full potential offered by the spectacular electronic and mechanical properties of graphene in applications will require extensive fundamental studies of the behavior of graphene in nanostructures and devices. We have a twofold aim: We will first seek to uncover the fundamental mechanisms that determine – and may limit – the potential of graphene in already foreseen optoelectronic applications. Second, we will start developing a next generation of graphene-based nanostructures for the development of electronic devices beyond CMOS. Research is needed to gain a detailed understanding of microscopic properties of defects in crystalline graphene, grain boundaries in polycrystalline graphene, or the influence of environment (such as various substrates), all of which affect the performance of mass-produced devices. Development of nanocircuits incorporating graphene nanoribbons and quantum dots will be essential to the exploit the new functionalities of graphene in high-end instrumentation and metrology. The study of 2D materials beyond graphene is key to enhance graphene’s properties by combining this material with monolayers of 2D crystals in superstructures, which will allow broadening of the range of functional applications of graphene nano-electronics in the long-term.

The activities in the first 30 months period will comprise

- Studies of electronic transport and optical properties in devices made of suspended single- and poly-crystalline graphene, investigation of the influence of substrate and functionalization of graphene on its transport properties, multiscale modeling of graphene-based structures.
- Spectroscopic characterization of graphene and defects in single- and polycrystalline graphene.
- Studies of thermal and mechanical properties of graphene, as well as graphene durability.
- Advancement of atomic scale technology in graphene, manufacturing graphene nanocircuits incorporating nanoribbons and quantum dots, and investigation of their quantum transport and dynamical properties.
- Implementation of graphene in metrology, for the development of fundamental resistance and current standards.
- Advancement of *ab initio* computation, high-performance computing for graphene studies, mesoscale modeling, further development of field theory and kinetic theory methods.
- Proximity-induced properties in graphene, including development of devices with electrically controlled superconducting properties.
- Production, characterization, and modeling of new 2D crystals beyond graphene: BN, hexagonal transition metal dichalcogenides.
- Assembly of hybrid structures and superstructures of graphene and other 2D materials, studies their lateral and vertical electronic transport properties, light emission and photovoltaics.

In WP3 Fundamentals, we shall study graphene produced in WP1 ’Materials’ and WP11 ’Production’. The newly developed understanding of fundamental limitations on graphene properties and insight into kinetic processes in graphene will be used in WP4 ’High-speed electronics’, WP5 ’Optoelectronics’, and WP6 ’Spintronics’. Performance of graphene in nanostructures and new routes developed for their enhancement will be used in WP8 ’Flexible electronics’, and WP5 ’Optoelectronics’. The newly developed technology will be provided to WP7 ’Sensors’.

3.4 WP4: High-speed Electronics

High frequency (HF) electronics, the core technology for modern information and communication systems, has been recognized from the very beginning as one of the most promising fields of application for graphene and related 2D materials, although facing strong competition from established technologies and also several scientific and technological challenges. Within this WP, the scientific and technological foundation for graphene based and enabled applications will be laid, by exploiting the unique properties of different 2D materials to create devices not conceivable with existing technologies. Different applications in the fields of data-communication, THz sensing and imaging as well as in the field of flexible substrates will be addressed.

The work plan for the 10-year period includes work on technology, devices, circuits and systems, with a vision to realize devices and systems based on graphene and related 2D materials (see figure below), which will overcome the performance limits of current state-of-the-art technologies. At the beginning the work will mainly focus on the technology and the component level to solve several challenges related to the unique properties of graphene and related 2D materials and also to explore the potential of novel device concepts such as ballistic or vertically stacked devices. A continuous extension to the circuit and system levels will be carried out, so that within the 10-year Flagship-Project not only demonstrators will be realized, but also their performance will be optimized towards the requirements of specific applications.

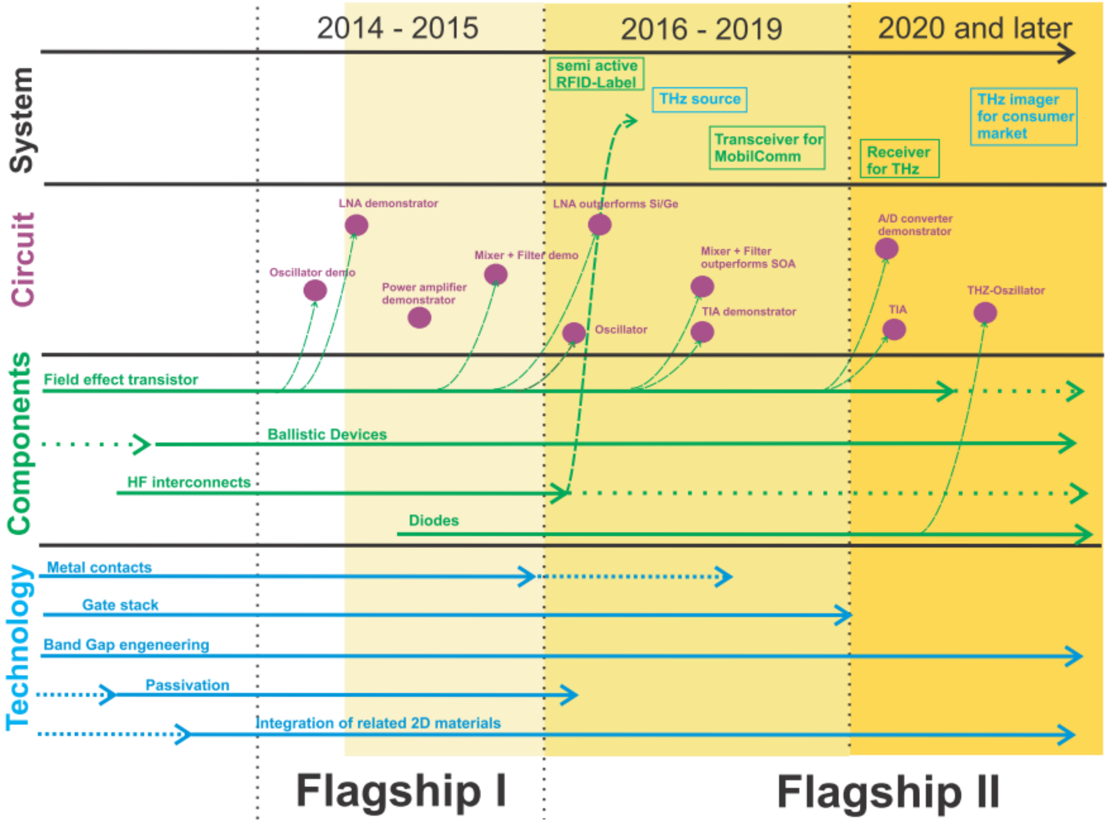


***Figure 6**: Work plan for the work package High speed electronics.*

The work within the first 30 month on the technology level will include minimizing contact resistance, band-gap engineering, integration of different 2D materials, gate stack integration and passivation using a joint experimental and theoretical approach. To ensure a smooth progress, theory will not only be utilized to reproduce the experimental findings but also to reduce the open parameter space by pointing out promising and also less promising routes. At the component level different device types required as building blocks for HF circuits and systems will be developed and further optimized. Already existing components like field-effect-transistor or interconnects are also in our focus as well as novel devices based on ballistic or tunneling transport and vertical heterostructues of different 2D materials. A device parameter library will be set up, which is essential for the realization of circuits based on those devices. On the circuit level, the work will concentrate on the realization of first demonstrators. Existing circuits design will be utilized and modified mainly at the beginning for incorporating existing components, while novel design paradigms will be set up to utilize the unique properties of components based on graphene and related 2D materials, given by the ambipolarity or ballistic transport. Demonstrator circuits to be realized within the first 30 months include mixers, low noise amplifiers, oscillators and power amplifiers.

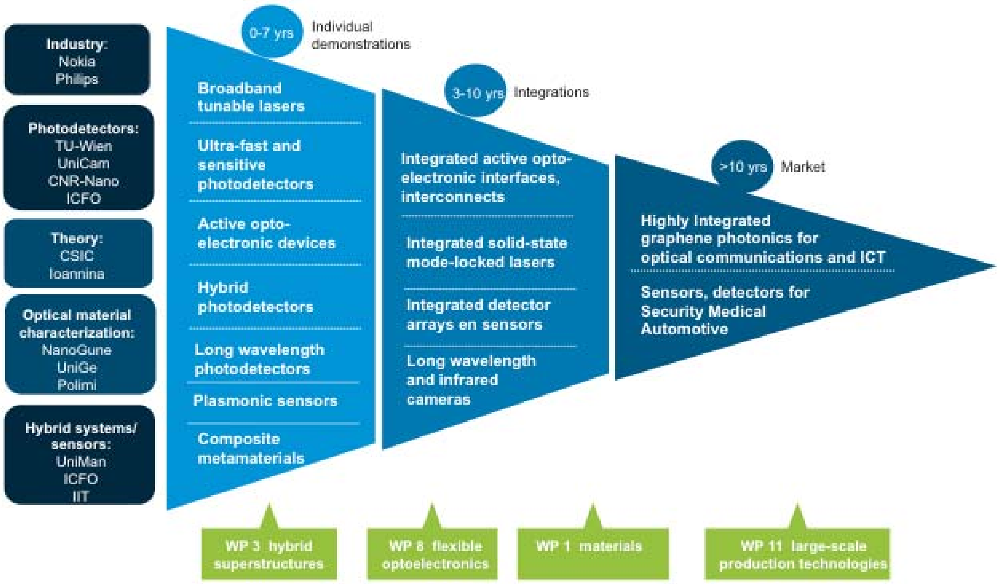
Collaboration with WP3 *Fundamental Science* will provide the scientific basis for realizing novel devices and for understanding the fundamental effects governing them, while the material platform required will be optimized within the WP1 *Materials*. Together with WP8 *Flexible Electronics* the foundations for flexible GHz electronics will be laid. The interaction with WP5 *Optoelectronics* and WP7 *Sensors* will concentrate on the realization of graphene based support circuits to further process the high data rates accumulated by specific devices.

3.5 WP5: Optoelectronics

Our goal is to establish a new field of graphene photonics, sustained by the convergence and co-integration of graphene-based electronic and photonic components such as lasers, optical waveguides, cavities, modulators, photodetectors, and solar cells. The unique optical properties of graphene, such as gate-tunable optical and plasmonic properties, saturable absorption, and broadband light absorption and generation, will enable novel functionalities, currently impossible with other materials. Graphene can be integrated with flexible and stretchable substrates, and its 2D-nature and compatibility with semiconductor processing platforms allows CMOS wafer-scale integrability and manufacturability. In contrast to many other nanotechnologies, the proposed WP offers the possibility for mass-production, which will be essential for the commercialization of future products.

We envision innovative technological applications in long-haul optical communications, inter- and intra-chip optical interconnects, wireless communications, security and surveillance applications, environmental monitoring, and energy harvesting. For this purpose, graphene, and related two-dimensional crystals and their hybrids, will be integrated with established and mature technologies such as dielectric (Si or plastic) waveguides, optical antennas, plasmonic structures (e.g. gratings or nanoparticles), quantum dots or semiconductors. We envisage the following applications to be developed within the next 10 years:

- Ultra-high bandwidth optical communications for ICT
- Wide-band tunable lasing
- Single-molecule detectors for medical applications
- Broad spectral-range cameras for medical, automotive and security applications
- Integration of graphene into a flexible and stretchable sensing platform for plastic electronics
- Large-scale detector arrays for low-cost and high-efficiency photodetection at infrared frequencies, based on hybrid graphene/semi-conductor systems, for safety and security applications in civil and military surveillance, night vision applications, automotive vision systems for driver safety, food and pharmaceutical inspection and environmental monitoring.
- Integrated and flexible photovoltaic systems covering the spectral range so far unused by conventional solar cells, with unprecedented efficiency for carbon-based devices
- THz imaging arrays and cameras that are compact, cheap, robust, fast, and display high sensitivity at room temperature.
- Highly sensitive and singe photon detectors for visible and near-infrared wavelengths, based on hybrid graphene/semi-conductor devices with photodetection gain.



For the first 30 months, the WP will be organized in the following tasks:

T1. Development of Graphene photodetectors (arrays) for visible and IR, with a focus on:

T1.1 High-speed electro-optical characterization

T1.2 Ultra-sensitive detection arrays based on graphene/semi-conductor or graphene/metal hybrid systems

T1.3 Co-integration with Si-based read-out circuits

T2. Development of graphene-based ultra-broadband tunable lasers. Integration into mode-locked lasers (fiber and solid state) to achieve ultra-broadband tunability in the telecommunications and mid-IR range.

T3. Implementation of graphene-based nanoscale optical routing and switching networks for opto-electronic interfaces and interconnects. This will exploit graphene as an active plasmonic material with ultra-strong and gate-tunable optical field localization. Interfaces between plasmon and optical circuits will be developed.

T4. Development of graphene-based tunable metamaterials. Plasmonic nanoresonators based on metallic/graphene composite materials tunable by relatively low voltages. The combination of graphene with plasmonic metamaterials will be exploited for ultrafast and small active optical elements for light-harvesting and sensing.

T5. Long-wavelength Photodetection. Plasmonic effects in graphene and the modulation of carrier transport in graphene channels will be exploited for resonant photoconductive detectors in the THz range. These will be compact, cheap, robust, fast, and with high sensitivity at room temperature.

T6. Active opto-electronics devices. High-speed, compact-footprint electro-optical modulators and switches integrated with Si waveguides or plasmonic circuits. The flexibility of graphene will enable integration with bendable substrates and plastic waveguides.

Graphene will be provided to this WP from WP1 Materials. For future integration of flexible optoelectronics with photodetection functionalities, collaboration will be established with WP8 Flexible Electronics. In particular, we will aim to jointly develop a new generation of active optical sensors and passive EM harvesters, operating in a wide spectral region from visible light to deep IR.

3.6 WP6: Spintronics

Among the potential candidates for spintronics, graphene, already acclaimed for its capability for more-than-Moore electronics, is very promising. Indeed, graphene could offer a true revolution for efficient spin manipulation and for the creation of a full spectrum of spintronic nanodevices for beyond CMOS technologies, while being compatible with more-than-Moore CMOS and non-volatile low energy MRAM memories. This WP aims at establishing the ultimate potential of graphene for spintronics, targeting efficient room temperature spin injection and detection but also spin gating and spin manipulation in graphene spintronic devices. By tackling this issue, we anticipate the development of external ways to control (gate) the propagation of spin currents, achieving operational reliability at room temperature and architectural compatibility with silicon technologies. Spin transport in graphene will be explored in different material systems, and by comparing the results in conjunction with realistic theoretical simulations, benchmarking graphene devices will be achieved along the way.

Over the 10-year period, the WP aims to design, engineer and address large scale manufacturability of advanced spintronic devices and architectures. Using the intrinsic molecular and 2D properties of graphene, the high-impact perspective is to combine the unique long spin lifetime and high mobilities with new paradigms to manipulate the spin information locally, towards a new generation of active, CMOS-compatible, molecularly-engineered spintronic devices, with possible low-energy operation. The explored concepts will use magnetic proximity effects, mechanical strain and molecular/atomic functionalization. The challenges will pave the way to all-spin-based information processing technology, with capabilities ranging from replicating conventional electronics, to quantum information processing, to advanced functionalities.

The activity in the first 30-months period will cover optimization of technological performances of graphene spin valve devices, including the spin injection/detection efficiency from magnetic contacts. Here we will focus on the specific role of the magnetic contacts, optimizing their spin injection and detection efficiency. Also their possible role in the spin relaxation and spin dephasing processes will be investigated. As a very important activity we will study and compare the role of the different graphene platforms (in particular the substrates) in the spin relaxation and dephasing processes. In particular we will make a detailed comparison between exfoliated graphene on SiO_2, graphene on boron nitride (BN), and graphene grown on SiC. The goal is to classify the material and device parameters which have to date shown limited spin transport. These results will be compared with spin transport and spin relaxation in suspended graphene devices, which will be used as a reference system. With a main focus on spin ensembles, the room temperature capability of graphene devices will be ascertained. The sensitivity of the graphene spins to other degrees of freedom, including other (localized) spins, phonons, mechanical strain (which could tune local spin-orbit coupling and spin precession) will be investigated together with their possible exploitation in sensor applications (magnetic sensing). We will investigate novel ways to induce (para-) magnetism in graphene, by introducing localized (defect) states in a controlled way or by decoration of the graphene surface with (magnetic) atoms or molecules. In the search for fingerprints of local magnetic ordering states and magnetoresistance profiles we will also target chemically modified graphene based materials, to envision the possibilities of new physical phenomena. The possibilities to induce ferromagnetism and/or spin-orbit interactions in graphene by the proximity of other materials (including ferromagnetic and ferrimagnetic insulators) will be endeavored, with the target to demonstrate and employ spin filtering effects. Finally we will compare spintronic system based on single layer, bilayer and multilayer graphene.

At the theoretical level, we shall develop an advanced spin transport simulation strategy based on a multiscale approach combining *ab initio* calculations with tight-binding models for material parameterization (material structures, defects, deposited magnetic oxides, ad-atoms and adsorbed molecules) with semiclassical or quantum transport methods for following spin diffusion. First-principles and tight-binding calculations of single layer and bilayer graphene covered with vacancies, hydrogen ad-atoms, magnetic molecules and deposited magnetic oxides (in the presence of external electric fields) will be performed, to establish the effects of spin-orbit coupling and magnetic interactions on induced spin relaxation and spin-orbit transport phenomena. Spin-dependent transport calculations will be achieved up to mesoscopic scale using efficient quantum transport methodologies (Kubo and Landauer in equilibrium and non-equilibrium regimes), with evaluation of transport lengths scales (mean free path, spin diffusion length, *etc.*) and transport tunability, providing guidance concerning spin relaxation mechanisms and gating efficiency of spin polarized currents in the chemically/structurally modified graphene devices.

A strong link will be established with WP3 Fundamentals, concerning the understanding of spin relaxation/dephasing studies in graphene nanostructures (nanoribbons and quantum dots) in the lower temperature regime. The physics of (localized) spins in graphene nanostructures will be compared with the spin physics in two-dimensional spin ensembles, with the aim of understanding the basic mechanisms which interact with the spins in graphene (hyperfine interaction, spin orbit interaction, electron phonon interaction). A very important interaction will be established with WP1 Materials, concerning the different materials systems in which spin transport and spin dynamics will be studied. Also for the characterization of the graphene systems we will collaborate intensively with other WPs.

3.7 WP7: Sensors

We anticipate that the Sensors work package will be primarily funded through the ERA-NET+ instrument. Therefore, the activities in the CP-CSA part of the Flagship are limited to a sub-category of nanoelelctromechanical sensors that are closely linked to the ICT-focused work packages. The ERA-NET+ instrument is intended to fund additional sensor types (*e.g.* chemical and biological), and sensors that target applications outside the ICT area such as environmental monitoring. Should the actual implementation structure deviate from the anticipated combination of a CP-CSA and an ERA-NET+, we will reconsider the contents and extent of this work packages.

Graphene membranes offer the ultimate potential sensitivity to tiny forces due to their extremely low mass. Graphene also has exceptional electrical characteristics, with extremely high room-temperature electron mobility. The combination of these two properties makes them ideal for sensors based on nano-electro-mechanical systems (NEMS). In this sensor work package of the graphene flagship we will explore the possibilities of exploiting (few-layer) graphene NEMS. State-of-the art measurements include optical read-out schemes operational at room temperature and electrical ones that are can be used in a wider range of temperatures. However, for applications the field is still in need of efficient transduction schemes.

In many applications, sensors are used to measure small electrical signals, forces or masses. Performance critically depends on an efficient coupling between the yet unknown signal and the measuring device. Due to their small sizes and corresponding small masses, graphene-based devices may offer such an efficient coupling as they should be very sensitive to external stimuli, which in combination with their high carrier mobility is highly appealing. The development of new detection schemes towards better sensors is expected to find applications in a wide range of fields (biosensors, chemical sensors or physical sensors). Several read-out schemes can be envisaged. Examples include electromechanical, optomechanical, optical, and electrical transduction schemes, which may also find a use in quantum information processing. In the coming 10 years, the challenge is to exploit the special properties of (few-layer) graphene associated with their small dimensions and their unique optoelectronic and mechanical response.

In the first 30 months of this program, we will explore three different complementary approaches to solving one significant challenge in implementing graphene sensors based on mechanical properties: the readout of the graphene displacement and the exploitation of the intrinsic nonlinearities in graphene resonators. At Delft, we will develop electrical techniques to read out mechanical deformation and motion of graphene NEMS at room temperature with a sensitivity approaching that limited by thermal (Brownian) motion. While the thermal motion limited detection of graphene membranes at room temperature has achieved using optical techniques, such techniques are not suitable for on-chip integration in NEMS sensors. To establish this, we will explore various sensitive on-chip readout techniques such as Silicon FET charge sensors and high-Q microwave resonant circuits. Doing so, we will implement on-chip scalable arrays of graphene NEMS sensors operating at the theoretical limit of the detection sensitivity. These devices may find application in, for example, NEMS microphones or sensitive gas detectors.

Modeling aspects of ultra-sensitive mass sensing will be the focus of the Chalmers group. An important figure of merit is the quality factor which is usually the limiting factor for obtaining a high mass sensitivity along with the phase noise. The main goal is to understand the role of thermal fluctuations, both mechanical as well as electronic, on the quality factor of resonators and on the noise figure. Of equal importance is to understand how the adsorption and motion of analytes affects the local mechanical properties of graphene. While detecting a frequency shift due to an added mass is enough for detection, Chalmers will also consider the effect of particles on the local mechanical properties, studies which also bear on the possibility to functionalize the graphene to target specific nanoparticles. The third aspect which will be taken into consideration is how the often strongly nonlinear resonant response of graphene resonators, leading to for instance bifurcations, can be used for achieving higher sensitivity in mass-sensing applications.

At the Center for Nanostructured Graphene at Copenhagen gas sensors will be built exploiting the change of electrical properties upon mechanical deformation. Graphene sheets will be placed on nanostructured substrates and will lie on the substrate like a carpet experiencing deformations determined by the interactions between graphene and the suitably functionalized substrate. These deformations will lead to a modified reactivity between the graphene and various gas atoms that the structure is exposed to. The corresponding change in the electrical response of the graphene can then be used to probe these interactions. Both experiments and extensive calculations of reactivity of graphene under various states of stress will be performed.

The Helsinki group will built a low-noise electromechanical microwave amplifier operating at low-temperatures, which is expected to reach the Heisenberg limit of lowest possible added noise. The amplifier is based on a suspended graphene membrane and can be set to be either phase sensitive or phase insensitive; in the phase sensitive case it would represent a simple and efficient alternative to nonlinear amplifiers such as Josephson amplifiers and converters or SQUID arrays, for the implementation of highly efficient, quantum-limited homodyne detection at microwave frequency. Scaling down with the dimensions, these amplifiers could also be operated at higher frequencies. By using mechanical mixing, these devices may facilitate radiation detection even in the difficult terahertz band. A further opportunity offered by graphene-based electromechanical devices is that they can be easily driven into the nonlinear mechanical regime.

It is to be expected that in the short term the closest interaction will be with the high-speed electronics work package, in particular concerning THz detection as there is a lack of sensitive detectors for this frequency range. Optoelectronics of graphene is an interesting direction as it can provide new means for sensitive read-out and transduction schemes. Furthermore, discoveries in the fundamental and spintronics work packages may lead to new detection schemes exploitable for sensing applications. On the somewhat longer time frame, when the working principle of sensing starts to be established, interactions with the Health and environment work package should lead to the design and fabrication of specific sensors.

3.8 WP8: Flexible Electronics

This WP is focused on the application of graphene to key enabling technologies required for the realization of flexible electronic devices and systems. Graphene has several unique electrical, mechanical and optical properties, which will enable novel applications as well as enhanced performance in printed and flexible electronics. The application of novel, graphene based solutions to printed electronics is expected to deliver benefits in terms of both cost advantage and uniqueness of attributes and performance. In this context graphene can be considered a truly enabling foundation for many technologies and as a flexible transparent semiconductor it is also the most natural choice for flexible (and possible transparent) electronics. Hence the main objective is to achieve a versatile graphene based technology platform for flexible electronic devices.

In the 10-year perspective, the vision for flexible electronics is built upon five key technology enablers (TE), which are then unified around two streams of applications. Key TEs are *T1 Fabrication and integration, T2 Energy, T3 Connectivity, T4 Sensing,* and *T5 Conductive Transparent Films.* The two streams of applications identified by industry are *D1 Smart Portable Devices* and *D2 Energy Autonomous Sensors*. This application driven structure allows an efficient and targeted use of the available R&D resources and also the delivery, over time, of a set of technically and business relevant demonstrators in each of the identified application stream.

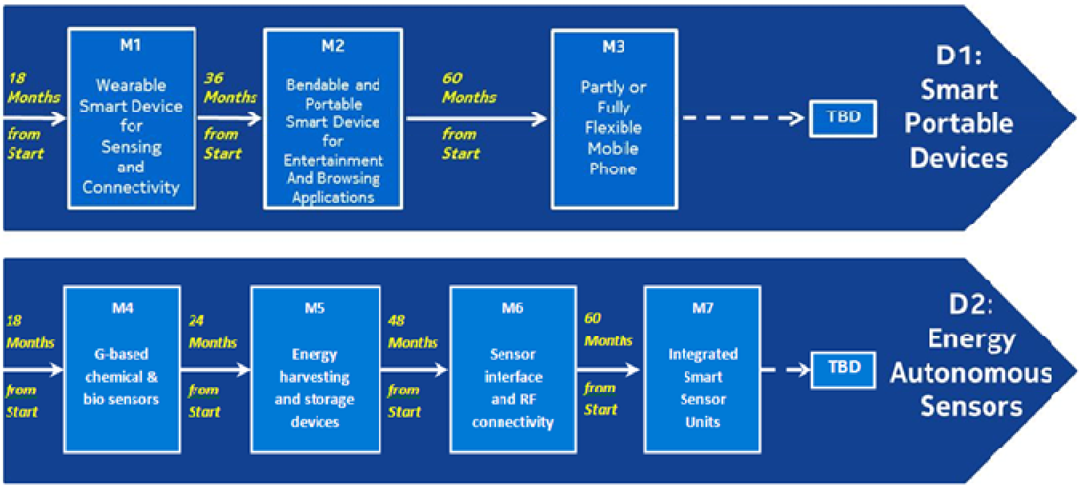


***Figure 7**: Two identified streams of applications targeted by the WP Flexible Electronics.*

In the first 30-month period, special focus will be in the increased maturity of the TEs listed above. The success will then be proven by first level application demonstrators described below. For instance different fabrication approaches will be developed such as printing of graphene inks, but also the scaling up the manufacturing of integrated components will be investigated. The work package addresses also the need for developing flexible versions of essential energy related technologies, but the flexibility creates also new requirements and opportunities for dedicated connectivity solutions such as radio communication. Biocompatible large area sensors and flexible version of these will also be one of the key technology enablers developed in this WP. Finally, electromechanical and reliability tests of individual layers, substrates, devices and full systems will be performed.

In the first **D1** (**"Smart Portable Devices"**) application stream we expect the following major prototype demonstrators to be realized: *Year 2: Wearable Smart Device for Sensing and Connectivity* – Leveraging both existing and new, graphene based technologies this demonstrators will show the potential for cost advantage and/or performance enhancement in wearable, connected devices for the emerging market fitness and wellness application. *Year 3: Bendable and Portable Smart Device for Entertainment and Browsing Applications* – Combining advanced material, energy, connectivity and integration/manufacturing technologies developed within the Flagship projects with display and logic processors from external suppliers, this demonstrators will showcase radically new solutions for game control and user interaction and manipulation of content. Year 4 and Beyond: Partly or Fully Flexible Mobile Phone – The most advanced and challenging demonstrator that can be envisaged at this stage will attempt to reproduce important functionalities of a smart phone in a partly or fully flexible format.

In **the D2 ("Energy Autonomous Sensors")** stream we expect the following major prototype demonstrators to be realized: *Year 2: G-based chemical and bio sensors* – Exploiting both existing and new sensing devices with high or ultra-high sensitivity and chemical stability, based on graphene functionalization chemistry, intrinsic biocompatibility and ambipolar characteristics of G-FET devices. *Year 3: Energy Harvesting and Storage devices* – Developing energy related technologies tailored for flexible substrates such as flexible batteries, super-capacitors and their integration with harvesting devices. This milestone aims to provide the "engine" to propel the autonomous sensor devices. Year 4 and beyond: Integrated Smart Sensor Units with RF connectivity – At first, we will combine RF device and circuit applications based on ambipolar non-linear graphene electronics for RF connectivity with Analog Sensor Interfaces, and integrating both on a flexible foil substrate. Finally, we will develop and provide the necessary infrastructure towards “graphene-augmented” smart integrated sensors on flexible substrates, with the necessary energy harvesting and storage capability to work autonomously and wireless connected to the environment.

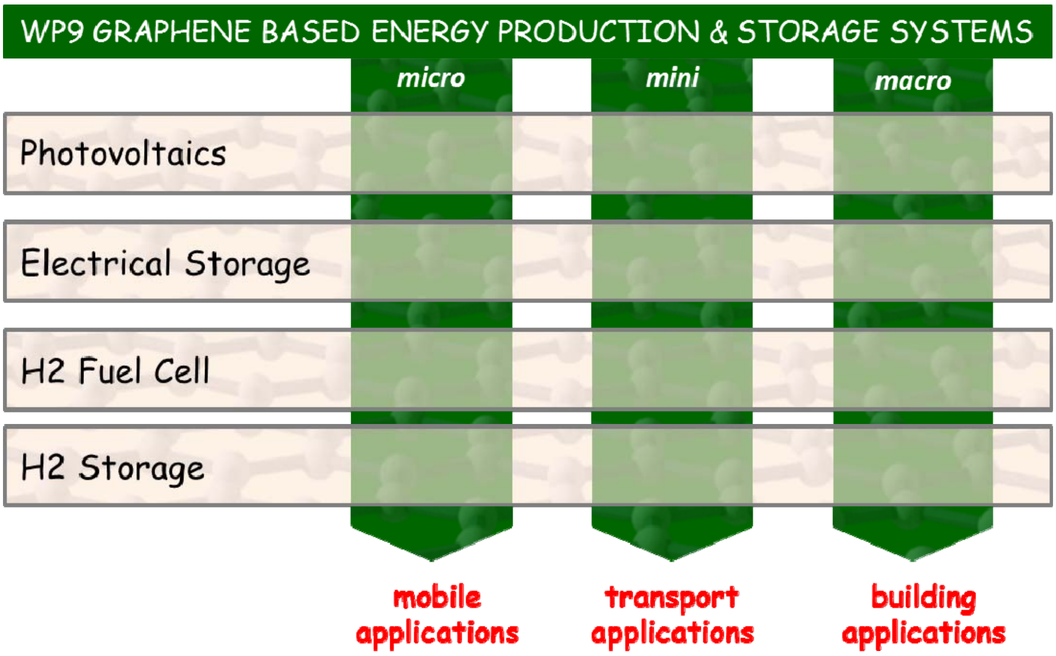
It is anticipated that all milestone prototypes are designed to benefit from the progress of both application streams.

This WP will have special focus on challenges and attributes related to flexibility and hence the close interaction with other parts of the project is crucial. The work will be made in a close collaboration with work packages WP1 Materials, WP11 Production, WP3 Fundamental Science, WP9 Energy, WP10 Nanocomposites, WP7 Sensors, WP5 Optoelectronics, and WP8 High frequency Electronics.

3.9 WP9: Energy Applications

Graphene is the material at the base of one of the most promising and versatile enabling nanotechnology addressing the *“secure, clean and efficient energy”* Horizon 2020 objective. Graphene has the potential to bring disruptive solutions to the current industrial challenges related to both energy generation and storage applications, first in nano-enhanced products, then in radically new nano-enabled products able to integrate different functionalities.

In the 10-year perspective, this application-driven WP will develop and demonstrate the industrial potentials of key enabling micro, mini and macro graphene-based systems for energy production (photovoltaics, fuel cells), electrical energy storage (supercapacitors, batteries) and hydrogen storage. In accordance with the GRAPHENE roadmap, the Energy WP will mix from the beginning short term/low risk and long term/high risk activities in order to maximize the scientific and industrial impacts along the project timeframe. We expect to deliver industrial-relevant proof-of-concept demonstrators. They will also measure the progress towards the targeted technology readiness levels required for industrial uptake. Research priorities will be steered according to these results.



In the first 30-month period, WP9 specific objectives are:

PHOTOVOLTAIC

- Inorganic PV: graphene transparent conductors on standard inorganic microstructured PV cells as an alternative to conventional TCOs; disruptive graphene nano-enhanced inorganic PV cells concepts (semi-transparent, 3D).
- Organic PV: atomistic description of light harvesting and electron transfer in graphene based organic PV; integration of solution processable graphene materials and hybrids in the active layer of organic PV cells; laser assisted graphene transparent conductors deposition on flexible substrates.
- Thin film PV: colloidal nanocrystals coatings on graphene sheets for improved visible and near-infrared light conversion efficiency.

ENERGY STORAGE

- Supercapacitors: demonstration of high electrolyte accessible surface area of graphene electrodes by simpler process routes that display performances that are beyond state-of-art; integration techniques on flexible substrates.
- Batteries: high energy and power densities graphene enhanced Li-ion batteries; feasibility of low-cost graphene-based printable battery electrodes.
- Identify promising disruptive routes for transparent supercapacitors and batteries.

FUEL CELL

- Functionalized graphene nanosheets with high surface area, low catalyst load, good electrical conductivity and chemical stability as a cost competitive solution to commercial carbon black as catalyst support.
- Feasibility of high performance, low noble-metal loading graphene based ultra-thin electrodes materials and evaluate their potential in fuel cells and redox-flow cells architecture.

HYDROGEN STORAGE

- Preparation of bulk graphene materials with high surface area. Functionalization of graphene layers by metal ad-atoms and molecular groups, making graphene-containing composite materials to achieve hydrogen uptake of 5.5 wt%. Demonstrate methods for the controlled uptake and release of hydrogen in graphene materials at fixed temperature and pressure. Reversible hydrogen storage in graphene materials within temperature and pressure ranges suitable for applications.

WP9 Energy will benefit from the latest generation of graphene synthesis and transfer techniques developed in WP1 Materials and WP11 Production, and will provide material and production specifications required for addressing the next generation energy components challenges. Work will also be made in close collaboration with WP8 Flexible Electronics that requires the integration of graphene based energy micro-systems on flexible substrates. Interaction with WP5 Optoelectronics is also envisaged to develop strategies to increase the absorption of visible light by exploring graphene surface plasmons as well as tailored metal and semiconductor nanostructures to enhance and control the coupling between light and graphene.

3.10 WP10: Nanocomposites

The 10-year vision for WP Nanocomposites is to transfer the ideal properties of single graphene sheets from the atomic scale to the meso-macroscopic level (continuous layers or bulk materials). This ambitious and long-ranged scientific and technological challenge originates from a simple but fundamental concept: *all* the superlative properties quoted for graphene (huge charge mobility, high Young modulus, high thermal conductivity, low gas permeability, *etc*.) refer to single, defect-free sheets of graphene, usually obtained by mechanical exfoliation, and suspended to avoid interaction with any perturbing substrate. In most applications, however, graphene layers composed of different crystalline sheets will be used, with properties inferior to those of single sheets. Charge and heat transport are perturbed at inter-sheet domain boundaries, edge defects act as electronic traps, and multilayer sheets easily split apart under mechanical stress, causing device malfunction or failure.

To gain a full understanding of the electrical, chemical and mechanical interactions of graphene sheets with one another and with different materials, we plan to use advanced scanning probe, optical and electronic techniques with tailored setups to observe the behavior of graphene based composites in situ and in real time, while the material is subjected to electrical and/or mechanical stress.

The modeling and control of graphene inter-sheet interactions, as well as the interaction of graphene with different materials, is an ambitious scientific challenge. However, this challenge will be addressed with particular attention upon the most promising technological end-uses of the materials developed in such a way to achieve a significant and clear impact for the graphene flagship and on society.

In the first 30 month period, we will study different types of graphene, evaluating the most suitable ones for different applications. A similar approach will also be used for other 2D materials. An important advantage of these materials is that, as opposed to other nano-materials, they can be produced cost-effectively on a large scale by either bottom up (atom-by-atom growth) or top-down (exfoliation from bulk) approaches. We will take advantage of this by comparing the performance of graphene growth by bottom-up techniques (*e.g.*, chemical synthesis, vapor growth) with graphene obtained by exfoliation in solution. Graphene functionalized using covalent and supramolecular approaches will be produced, with the goal of improving sheet processability, sheet deposition on different substrates and dispersion in different bulk materials. Chemically modified graphene can be viewed as a 2D polymer containing extended aromatic frameworks and multiple functional groups. These groups shall be used for the covalent attachment of organic and inorganic nanoparticles including metal and metal oxide nanoparticles, forming 2D layered nanocomposites that have attracted great attention due to their unique catalytic, magnetic, biological, and optical properties.

Advanced scanning probe, optical and electronic techniques with tailored setups will be used to visualize, on the microscopic scale, the process of electrical/mechanical failure, and to find new ways to improve the materials' properties. In parallel to nano-scale characterization and modeling, the mechanical/electrical properties of the different graphene-based materials will also be characterized on the macro-scale by conventional procedures, and the materials will be incorporated into real working devices that shall include, but not be limited to, transistors, power electronics, transparent coatings for photovoltaics or displays, embedded sensors for mechanical failure or leak detection, light structural and functional materials for automotive and aerospace components, sensorized plastics for electro-domestic appliances.

The activity of the Nanocomposites WP will have strong interactions with all the other WPs of the flagship; in particular, exchange of knowledge, information and materials is foreseen with

WP1 Materials (2D materials, graphene nano-ribbons, molecules for graphene functionalization), WP8 Flexible Electronics (providing materials for flexible displays, touch screens, strain sensors, *etc*.) and WP5 Optoelectronics (exchange of know-how for characterization, optical properties of composites, evaluation of optoelectronic applications).

3.11 WP11: Production

The work package on Production will be closely aligned with the project(s) funded through the call ***NMP.2013.4.0-1*** on large scale production of graphene. Therefore, the work package will receive only limited funding from the CP-CSA instrument, and the bulk of the funding is expected to come through the NMP program. The primary target of this work package during the ramp-up period is to align the large scale production activities with other parts of the Flagship.

The 10-year vision of WP Production is to set up an efficient supply of high-quality graphene for a wide range of applications with a wide spectrum of specific material requirements. These areas include flagship targeted applications in ICT, energy, sensing, and advanced or light-weight materials, as well as in currently unforeseen future needs in other areas.

In the first 30-month period, the work within WP Production will be split into 3 key areas, namely

- graphene equipment,
- film production,
- bulk production.

Graphene equipment targets the needs of end applications which require the deposition of graphene onto substrates as part of the manufacturing process; examples of this are semiconductor processing such as the manufacture of integrated circuits or RF transistors. Graphene films are used in applications which utilize the graphene as part of a functional substrate, such as transparent conductors or sensors. Finally, bulk graphene in the form of a suspension/powder are used in applications such as composites.

The Production WP will interact with the rest of the flagship consortium to understand future requirements for graphene equipment, graphene films and bulk graphene, and will be able to exploit results of the consortium in terms of new synthesis recipes, transfer technology or applications. The Production WP, in collaboration with WP1 Materials will contribute a sufficient number of samples to research partners who do not have the capability to produce graphene in house.