



Conference series "The Big Six –
Spotlight on the EU-Flagship-Initiative"

Summary of the Conference "Exploring the Potential of Graphene"

by Hans Rudolf Ott,
chairperson of the SCNAT-"Platform Mathematics, Astronomy and Physics"

Organisation: SCNAT and SATW
Location: Sorell Hotel Ador, Bern
Date: March 8th, 2012

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Swiss Academy of Sciences
Akademie der Naturwissenschaften
Accademia di scienze naturali
Académie des sciences naturelles

SATW

Schweizerische Akademie der Technischen Wissenschaften
Académie suisse des sciences techniques
Accademia svizzera delle scienze tecniche
Swiss Academy of Engineering Sciences

General Summary

The conference was organized as part of a series of meetings, initiated and organised by the Swiss Academies of Arts and Sciences (swiss-academies), that aimed to satisfy the need for information of the Swiss scientific community on the high-priority projects of the EU-Flagship-Initiative. These projects received much attention in Swiss daily newspapers and weekly magazines, mainly due to the remarkably high profile of Swiss-based researchers in some of the six projects that survived the first round of review. In view of the enormous magnitude of human and financial resources involved, the Swiss Academies considered it necessary that the Swiss scientific community should be offered to learn more about the scientific contents and aims of these projects which are still on the list of the EU-Flagship-Initiative. This particular conference focused on the project “Exploring the Potential of Graphene” and included presentations, questions and discussions.

An amazing development of the physical appearance of carbon started in the mid 1980s with the discovery of large cage-type carbon molecules of which the best known C₆₀ is just one example. Subsequent work led to the realization of different varieties of carbon nanotubes with diameters in the range of nanometers, exhibiting amazing mechanical and electrical properties. More recently, successful realizations of sheets of single layers of carbon atoms, termed graphene, of lateral sizes from mesoscopic to macroscopic scales were reported. Apart from the genuine scientific interest in the particular physical properties of such atomically thin carbon layers – some of which were predicted by theory – it soon turned out that these objects also promise a high potential for a great variety of applications. From this point of view, the intention to initiate a special programme for exploring the potential of the new material graphene at the European level seems rather reasonable, if only scientific arguments are considered. However, in view of the expected investment of large amounts of human and financial resources and the enormous size of the project for this kind of topic, some questions regarding the rationale and the setting of the programme need to be answered as well.

Invited speakers were chosen to eventually cover the most important aspects of the project's topic. A majority of the presentations concentrated on the physics aspect of graphene in several ways. The chemistry of graphene and other carbon materials as well as first experiences and plans in the industrial sector were the topics of two additional lectures.

Summaries of the Presentations

Speakers (following the sequence of the presentations):

Jari Kinaret (spokesperson of the project), Chalmers University of Technology, Gothenburg, Sweden

Graphene-Based Revolutions in ICT and Beyond – an FET Flagship Proposal

In his role as the leader of the project, Kinaret devoted his presentation to explaining the reasons for implementing such a programme and to describing its aims and expected outcomes. In short, the general goal of the project is to create a focused community, based on bundling numerous existing or planned national programmes, to exploit the unique properties of graphene and related two-dimensional materials towards creating technical innovations and boosting economic growth. The main areas in which applications based on properties of graphene are seen include ICT (consumer and high-performance electronics and photonics), materials (ultralight and high-yield materials, novel electronic links), energy (small-size high-energy density batteries and capacitors) and health (biosensors, DNA sequencing). The rapidly growing research interest in graphene and its use in the last few years shows in an almost exponential growth of scientific publications and patent applications worldwide. In Europe alone, about 500 research groups in 29 countries are active in this field of research and more than 60 large companies seem to be involved in developing applications based on graphene. Activities in Europe are based on national and EC funding, currently reaching levels of more than 60 M €/y. While the number of scientific publications originating in European laboratories equals that of the corresponding outputs in both Asia and North America, the latter two regions clearly dominate regarding the number of patent applications. This situation obviously calls for a correction if the aim of implementing innovation and creating economic growth in Europe, based on graphene, is taken seriously.

Some information was given on the planned implementation of the programme. It involves several channels of the European funding system but also depends on significant nationally-based funding. The membership in the consortium of R&D partners of the programme is limited and can be obtained via a competitive application and selection procedure. A scientific panel with representatives of both the academic and the industrial sector will coordinate eleven R&D work packages. The coordination between knowledge driven research and development of technical applications will require major efforts in management. The general principles of governance were mentioned, however, it remains to be seen whether this enormous enterprise involving both academic and industrial cultures is manageable in this way.

Klaus Ensslin, Federal Institute of Technology Zurich, Switzerland

Graphene Quantum Circuits

The presentation started with an overview of existing graphene-related research in Switzerland, which is mainly based in Geneva, Lausanne, Basel and Zurich and involves groups with either experimental or theoretical activities in physics, chemistry and engineering. With respect to coordinated national efforts, research on graphene already is one of the topics in a recently established NCCR (Quantum Science and Technology, QSIT) and is foreseen in a proposal for a new NCCR (Carbon) dedicated to engineering applications based on carbon nanotubes and graphene.

The so-called quantum technology is based on artificial physical objects of sizes in the nanometer regime. Their physical behaviour is dominated by quantum effects. A typical object of this kind is a quantum dot where single electronic charges and spins can be manipulated. A major application of these objects is seen in so-called qubits, i.e., basic units of quantum computers. At present such nanounits are realized in specially tailored semiconductor structures. In monolayer graphene, the motion of charge carriers (electrons or holes) is strictly confined to two dimensions and therefore characteristically different from that in the mentioned semiconductor structures. By exploiting the special electronic properties of graphene, the fabrication of qubits of a quality that is significantly superior to the presently available devices is anticipated. Similarly, simply because of the genuine properties of carbon, the realization of a so-called spin qubit based on two quantum dots appears to be much more feasible by using graphene rather than semiconductor-based structures. The technical procedures for producing suitable semiconductor systems, mainly based on GaAs, and for the subsequent fabrication of nanostructure units are quite mature and routinely employed. Analogous procedures for producing qubits on the basis of graphene, however, remain to be developed.

Ensslin continued by briefly sketching some experimental achievements of his group at ETHZ towards the realization of versatile graphene-based qubits. The patterning of graphene on SiO₂ templates with Si backgates for tuning the electronic conduction of the sample's material has been successful and expected results have been verified. In a further step, nanostructures based on graphene were fabricated and their performance as quantum-dot devices was tested. Single-electron transistors based on graphene are feasible. In addition, single particle states and Landau levels in external magnetic fields were identified and various relevant energy scales were evaluated. These results indicate that graphene nanostructures can be produced with existing technical procedures. They also show that charge and spin degrees of freedom are accessible and can partly be manipulated. The realization of useful devices that may replace analogous semiconductor-based quantum circuits remains challenging and requires future efforts.

Klaus Müllen, Max-Planck-Institut für Polymerforschung, Mainz, Germany
Is the Future Black? The Chemist's Search for Graphene and Carbon Materials

This presentation was dedicated to summarising aspects of the chemistry and, in view of achieving a robust technology for applications, material's synthesis of graphene and related carbon structures. First attempts to grow very thin carbon sheets date back to the early 1960s when carbon-oxide reduction in suitable solutions resulted in single-atom lamellae of carbon. Although 15 years later, graphene was grown on metal surfaces, the transfer of such sheets onto other metal surfaces was achieved only much more recently. Using hexagonal carbon rings as a starting point, it is possible to build molecules in the form of chains, discs and spheres. In the present context, the two-dimensional (2D) variety is of main interest. Five different characteristic 2D graphene molecules have been identified up to now.

First, various routes to obtain 2D carbon layers from 3D carbon were discussed and device-oriented electronic performances of a particular 2D combination of molecules were presented. In particular it was shown how the band gap can be controlled by choosing the size of stable molecule assemblies. With respect to device fabrication, the possibilities to use self-assembly are being explored. There are two options. The first is the alignment of molecules from solution and the second is based on the macroscopic control of order from melt and solution via zone casting and zone crystallization. Müllen also presented examples of devices with a potential for electronic and medical applications obtained by self-assembly on the basis of other materials. Following this, the potential of carbon-based solutions in energy technology was discussed. Carbon nanospheres for the storage of Lithium in batteries served as an example. Graphene-based Li storage may be based on graphene-encapsulated nanoparticles of transition-metal oxides. First encouraging results with respect to electrochemical performance factors were presented. Since graphene has a high potential for applications using transparent, electronically conducting sheets, its use in combination with solar cells or light-emitting diodes is evident. A promising way of graphene production is given by the reduction of layered carbon oxide in a water solution. Chemical or thermal reduction allows easy synthesis and processing, resulting in high yields on large scales and therefore in low costs.

Finally, Müllen addressed one of the crucial problems concerning the future importance of technical applications of graphene. Although the mechanical exfoliation from bulky single-crystalline graphite using scotch tape results in single-crystal quality samples for investigating basic physical properties, this technique cannot be the solution for preparing technologically relevant graphene material. The low yield and the random size of the resulting samples are the main obstacles. An alternative is the corrugation-assisted mechanical exfoliation from few-atomic-layer carbon sheets deposited on corrugated Silicon substrates. For electronic applications, so-called graphene nanoribbons, which are prepared using zigzag polyphene-

nylenes as precursors, may serve as the starting material. What is attempted in this and other ways is to prepare graphene sheets of single-crystal quality with chemically-controlled procedures. One-atom thick layers of carbon, acting as membranes with large pores, may be used as filters in fuel cells or serve as separators in gas sensors.

Vladimir Falko (member of the projects graphene road-map team),
Lancaster University, UK

Graphene Flagship

The presentation emphasized that the project aims at broadening the knowledge basis on graphene and 2D materials beyond graphene. Ideas on how to combine science and technology on the basis of these materials are summarized in a road map. The road map recommends developing a flexible platform for the implementation of multifunctional materials in a broad range of applications with the prospect of commercialisation. Achieving this goal requires the participation of many disciplines in research and development, including different fields of both basic sciences and engineering.

Falko continued with an overview on opportunities that are offered by using graphene as a base material. From a long list, some examples were briefly mentioned, including flexible optoelectronics, transparent conductive coatings, optoelectronics and photonics in a broad sense, micro- and nanoelectronics using hybrid systems of C-MOS. After a brief discussion of the case of bilayer graphene, some other applications in high-end instrumentation, sensors and the energy sector were outlined. As mentioned before, all these uses evidently require robust production procedures with highly controlled processes suitable for mass production. At present, the quality of graphene samples can be tested *à posteriori*. The much more important *in-situ* quality control methods during production are not yet available; ideas how to accomplish this exist but their practical realisation still requires extensive R&D work. Significant research efforts are also required for developing hybrid- and superstructures involving graphene and other metallic or semiconducting 2D materials, based on new approaches regarding the creation of such structures and the exploitation of their functionalities.

The roadmap envisages that the attempted goal, i.e., the provision of consumer products between 2020 and 2025 will be achieved via two merging routes. Based on the understanding of properties and processes, in collaborations between academia and the private sector, new devices will be developed and prototypes realised. In parallel, the development of manufacturing processes and mass production processes will be pursued. At present, it is not quite clear how exactly the merging of the two routes will be achieved.

Alberto Morpurgo, University of Geneva, Switzerland

An Experimental Tour through some of the Unique Properties of Graphene

Following the first successful exfoliation and transfer of monolayers of graphite (graphene) and the subsequent demonstration of their gate-controlled electrical conductivity by Novoselov and Geim in 2004, a large number of experiments were carried out to explore the physical properties of graphene. Morpurgo's lecture aimed at summarising the particular aspects of electron motion in graphene and at illustrating some of the recent successes in graphene research with outstanding results and their implications.

As already mentioned in Müllen's contribution, the simple mechanical exfoliation using the scotch-tape method obviously has its limits and other methods to fabricate graphene of adequate size and quality have to be developed. First successes were achieved via CVD of carbon on metal substrates, stabilizing the graphene structure with a polymer layer and removing the substrate by wet etching. By means of this method, square-meter-size foils were produced. The number of atomic layers of a foil can, in retrospect, be determined by optical methods.

An early encouraging result indicating the great potential of graphene for electronic applications was the temperature-independent high mobility of charge carriers, an order of magnitude higher than in common Si-based integrated circuits operated at room temperature. This implies defect-limited ballistic transport of electrons or holes on the micrometer scale. The amazing low density of defects provides opportunities in sensor applications. The deposition of molecules on graphene structures may, by charge transfer, induce electronically-active defects whose presence provoke measurable variations in resistivity. Thus, the method appears to provide a feasible option for single-molecule detection with a broad range of applications.

Most of the amazing electronic properties of graphene are related to its particular electronic excitation spectrum. For strictly 2D, monolayer graphene, the $E(k)$ spectrum is gapless and $E \sim k$. Close to the meeting point of the inversely arranged cones of $E(k)$, the excitations have zero mass and other unusual properties, and can be described with the Dirac formalism of relativistic quantum mechanics. This situation changes significantly for bi- and trilayer foils of which the band structures $E(k)$ to some extent exhibit conventional features but can be tuned by gating. In this sense, the electronic properties of graphene can, quite generally, be tuned by choosing the number of layers and gating. The latter also allows for controlling the number of occupied states in the electron and hole channel, respectively. Gapping in $E(k)$, required in many applications, can also be obtained by nanostructuring the material. It is expected that in this way, tuneable light sources in the range between THz and infrared can be obtained. A variety of recently published

experimental results demonstrate the tunability of the band structure by exploiting the mentioned possibilities.

In summary, many experiments by different groups have demonstrated that graphene and its derivatives are likely to open up new opportunities for improved or new applications. Already known in this respect are transparent electrodes, molecular sensors, high-frequency switching, light sources and other photonic devices and composite materials.

T. Hintermann, BASF-The Chemical Company, Basel, Switzerland

Graphene Technology Platform at BASF

According to the roadmap presented by Falko, the project is based on a considerable interaction between academia and industry during the entire duration of the programme. Therefore, it seemed of interest to complement the conference's programme with a contribution of an industrial stakeholder covering the status of, and future plans for graphene-related research and development in the private sector. It proved rather difficult to find a representative from the industrial sector. Most of the known current efforts in industry seem to concentrate on the materials' preparation sector.

A brief introduction of BASF as a world-leading chemical company with a broad portfolio of activities in many sectors was followed by the presentation of a list of the company's principal plans for innovation in five growth clusters. Graphene research and development with short- medium- and long-term perspectives is indeed on the agenda of BASF's future activities. Not surprising, the synthesis of graphene is currently of high priority. Two routes are followed. The first aims at the production of graphene from carbon in general, the second focuses on particular synthesis procedures adapted to given applications. The company's interest follows the forecasts of addressable markets for special new materials, i.e., graphene in this case. The most promising end-user applications are conductive inks, semiconductors and energy storage with a total market value exceeding 10⁹ \$/y in 2020.

Since 2008, BASF is engaged in various sectors of graphene research and development. They include conductive ink for printable electronics, basic material in car-construction applications, polymer composites for thermoplastics, improvements of Li-ion batteries (energy storage) and graphene nanoribbons for carbon-based semiconductor applications in optoelectronics and molecular electronics. The company expects to identify other relevant fields for industrial applications of graphene in the future.

Round Table

The conference ended with a brief round table discussion, moderated by Øystein Fischer of the University of Geneva. The round table included the speakers of the conference, the chairpersons of the SCNAT platforms for Chemistry (Karl Gademann) and Mathematics, Astronomy and Physics (Hans Rudolf Ott), respectively as well as Oliver Gröning of EMPA Dübendorf. From a scientific point of view, the project is not really controversial. Accordingly, the discussion concentrated on general aspects of the chosen approach to reach the declared goals and on the degree of involvement of the concerned Swiss communities in academia and industry.

Conclusions

The conference made it clear that the envisaged project will not be a large research programme of the usual type, i.e., knowledge driven. Instead it is, already at the outset, economy driven to a large extent. The clear goal stated in the road map is to provide consumer products and thus economic benefits for Europe. To reach this goal, considerable efforts in research and development are a prerequisite. Basic research in physics, chemistry and materials science, mechanical engineering and electro engineering as well as computer science and biology, will have to be coordinated by means of technical measures in the production of suitable starting materials, device developments and manufacturing. Thus, a close cooperation between academic research and industrial development from the very beginning is indispensable. An efficient and successful management of the project will require balancing the efforts between the partners in academia and industry, first within each community and second across their borders. This is a major and difficult task. It is not clear from the presentations of Kinaret and Falko, whether the corresponding plans for managing the programme are adequately adapted to the task.

Graphene and its derivatives are, no doubt, materials that have great potential in applications that are already known. Hopefully, their use will also initiate new ideas of applications and lead to yet unexpected inventions. There is a lot of room for knowledge-driven research. As is common practice, the selection of participants in this part of the programme can be based on internationally accepted quality conditions for proposals of this kind of research. Comparing the degree of interest in this research community with the plans for the realization of the project presented during the conference, the rejection rate will be enormous. It is much less clear, however, how industrial partners will be selected. Industries tend to follow their own interests and it may prove impossible to control their activities within an international collaboration of the envisaged size. It is almost certain that the industrial sector will need to invest much more human and financial resources than the academic sector. The final project application should be much clearer on this point and offer robust solutions.

Concerning the Swiss participation in the project, there is no doubt that the related research community based at several Swiss Universities and research laboratories is well prepared for the participation in the programme. It would definitely be able to provide significant, purely scientific contributions. As mentioned in the introduction of this report, a few Swiss national programmes cover at least parts of the type of research that is envisaged here. There is much less clarity about the interest and possible participations of the industrial sector of Switzerland. Although the speaker representing the industrial sector is based in Switzerland, his employer BASF is an internationally active firm, which represents neither Switzerland nor Europe. In view of the participation in the conference, it is clear that the interest of the Swiss-based researchers in the academic sector in participating in the programme is much higher than that of Swiss industrial firms.

The Big Six – Spotlight on the EU-Flagship-Initiative

The Swiss Academies of Arts and Sciences organized the conference series “The Big Six – Spotlight on the EU-Flagship-Initiative”, aiming to inform the Swiss scientific community about the planned EU projects. The meetings provided a platform to discuss both general and specific questions concerning the potential, ambitions and trends and helped to form an opinion on the priority of a Swiss participation in such programs:

- **Perspectives of High Power Computing in Neurosciences**, 20 January 2012, Bern
- **Exploring the Potential of Graphene**, 8 March 2012, Bern
- **Medicine in the 21st century: IT as a magic bullet**, 16 March 2012, Bern
- **Participatory Computing for our Complex World**, 21 March 2012, Zurich
- **Guardian Angels for a Smarter Life – innovations enabled by Zero-Power technologies**, 17 April 2012, Zurich
- **Rise of Sentient Machines? Robot Companions for Citizens**, 22 May 2012, Bern

Further information: www.akademien-schweiz.ch/flagshipseries