Taking novel materials from concept to application

The extraordinary electronic properties of graphene have generated great interest in both the academic and commercial sectors, with scientists predicting the material could be used in a wide range of technological products. However, many challenges remain before graphene can be widely applied, says **Professor Oleg Yazyev** of the EPFL in Lausanne, Switzerland

The development of graphene, a two-dimensional material formed by a single layer of carbon atoms, has generated great interest in both the academic and commercial sectors, with scientists predicting that it could in future be applied in everything from consumer electronics to solar panels. However, many outstanding problems must be solved before these predictions can be fulfilled, an area which forms the primary focus of Professor Oleg Yazyev's research. "The global objective of my research is to solve problems on the way from the basic physical properties of novel electronic materials to their technological applications," he says. Based at the École de Polytechnique Fédérale de Lausanne (EPFL) in Switzerland, Professor Yazyev's research group is studying the novel physical properties of graphene by means of theory and computations. "Charge-carrier mobilities in graphene are exceptionally high, which makes it very interesting for making high-speed electronic devices," he explains. "However, graphene is very different from the materials which are currently used in electronics. It presents us with a large number of new problems which we still have to solve before we see the first graphene computer."

Understanding wafer-scale graphene

Among the most important problems is the difficulty of controlling charge transport. Today graphene can be produced at both wafer scales and beyond, but scaled-up samples do have a different structure to micrometre flakes, which are often single-crystalline in structure. "At larger scales graphene is unavoidably polycrystalline, meaning it's composed of single-crystalline domains with different relative orientations of the crystalline lattice," explains Professor Yazyev. Topological defects like grain boundaries, line defects which separate two-dimensional single-crystalline domains, are intrinsic to polycrystalline materials and have a significant impact on the electronic properties of graphene. "Studying polycrystalline graphene and relevant topological defects is an important project in my group. I'm particularly interested in understanding how these defects affect the electronic transport properties of graphene," says Professor Yazyev. "We are also trying to propose new concepts for using these defects to control electronic transport in graphene, as functional components of nanoelectronic devices. This research is directly relevant to the potential technological applications of graphene, especially in electronics."

During transport charge carriers pass through a grain boundary with a certain probability. This transmission probability varies according to several factors. "It would depend on the energy of the charge carrier, on the direction it travels in respect to the grain boundary, and of course on the characteristics of the grain boundary itself. These include the relative orientation of the two single-crystalline domains and the local atomic structure of the grain boundary. There might also be some other interesting phenomena; for example, we have predicted theoretically that grain boundaries of certain structural types completely reflect charge carriers in certain energy ranges," says Professor Yazyev. Such defects could in principle be used as device components, utilising properties not present in single crystalline graphene; Professor Yazyev says this is a technically challenging area. "If we want to use these defects for a purpose, as device components, we need to learn how to engineer them," he explains. "This is a very challenging task – currently there is no method which really demonstrates a sufficient degree of control over the structure of these defects. Developing such a method is one of the goals of my research."

This hints at the wider commercial potential of graphene, and also the scope for further research into the material and its possible applications. With such a wide range of research possibilities, Professor Yazyev doesn't want to limit himself to looking at just polycrystalline graphene. "There are some other new ideas which may find use in technology, such as manufacturing one-dimensional graphene nanostructures," he says. Professor Yazyev has clear plans for the future. "From understanding electronic transport in polycrystalline graphene I would like to move on to the transport properties of self-assembled graphene nanostructures produced in a bottom-up chemical approach, which could be a highly effective method for making functional nanodevices at large scales," he outlines.

While his research is mainly theoretical in nature, Professor Yazyev maintains close relationships with experimental colleagues and is keen to work in areas that could be relevant to the potential commercial applications of graphene. "We are actively

using the results obtained by our experimental colleagues. We collaborate with them in helping to understand their results, and, most importantly, we are trying to motivate them to realize our theoretical predictions in practice," he outlines. "We can accurately predict how various types of structural modifications change the properties of graphene. This includes specific electronic, magnetic, transport, mechanical and optical properties. And by combining our efforts with experimentalists we aim to introduce graphene into real technological applications sooner."

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Beyond traditional electronics

Alongside its focus on applying novel materials in traditional electronics, the group is also working on alternative technologies. One such area is spintronics, an extension of electronics which makes use of electron spins to store and operate information. "The idea is to combine the extraordinary electronic properties of graphene, which is what makes it exciting in terms of pure electronics, with magnetic ordering to produce an ultimate platform for spintronic devices," explains Professor Yazyev. "We would like to have magnetic ordering at least at room temperature, the regime in which practical spintronic devices are supposed to operate."

The group is also pursuing research into other Dirac fermion materials; prominent among these are topological insulators, which display Dirac fermion surface states similar in many ways to those in graphene. However, these materials present a number of new physical properties, such as the absence of spin degeneracy and the helical spin texture of the Dirac fermion surface states. "Topological insulators realise the intrinsic electronic topological order. This is a whole new class of materials found only very recently. I would compare the discovery of topological insulators to the discovery of superconductivity. This is basically of the same calibre," says Professor Yazyev.

"I'm actively extending the scope of my research interests into the field of topological insulators as the field grows, in particular I would like to focus on the inter-disciplinary aspects. Most of the research in this area is currently being done by the physics community, but there are also many exciting problems related to materials science, chemistry and electrical engineering."

Artistic image of the atomic structure of a grain boundary in graphene

At a glance

Full Project Title

Dirac fermion materials: from fundamental science to applications through computation

Project Objectives

The projects aims at understanding and designing novel materials, functional nanostructures and devices in silico, that is, by means of computer simulations involving various level of computational complexity. The ultimate goal is to build a continuous bridge between fundamental science and technological applications based on numerical experiments.

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Professor Oleg Yazyev gained his degree in chemistry from Moscow State University in 2003 then joined Ecole Polytechnique Fédérale de Lausanne (EPFL), completing his PhD thesis in chemistry and chemical engineering in 2007. His current research focuses on the theoretical and computational physics of the recently discovered Dirac fermion materials with a strong emphasis on their prospective technological applications.

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