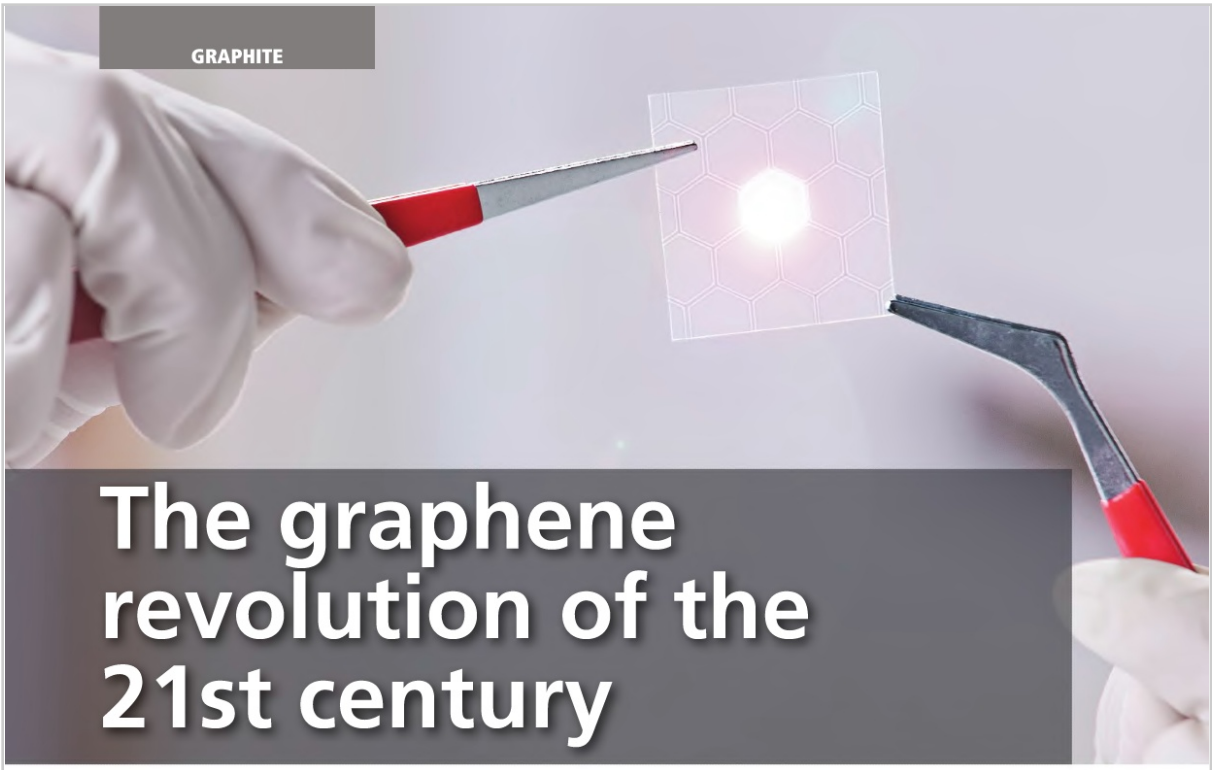

The graphene revolution of the 21st century

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When it comes to exciting new materials for technological and industrial applications, graphene is one of the most promising.

Graphene was discovered at the beginning of this century by Andre Geim and Konstantin Novoselov at the University of Manchester. The discoverers were awarded the Nobel Prize in 2010 (and a knighthood shortly thereafter).

Graphene is an atom-thick two-dimensional (2D) material composed of sheets of pure carbon. Remarkably, it was first produced by applying adhesive tape to graphite, then repeatedly sticking the tape to itself until just a monolayer of graphite remained. Seriously, it's that simple! The tape dispenser and the lump of graphite are now displayed at the Nobel Museum in Stockholm. Prior to this discovery, graphene had eluded chemists and physicists for many years. In fact, it was believed that a 2D form of carbon could not exist because it would be thermodynamically unstable compared with other forms of carbon, such as graphite, fullerenes, and nanotubes. Soon after the discovery of graphene, it was realised that the material bears not only academic significance, but that it also has exceptional physical, optical and electrical properties. For example, graphene is the thinnest possible material, is roughly 200 times stronger than steel, weighs less than one milligram per square metre, and has a higher electrical and thermal conductivity than copper.

In addition, graphene is remarkably flexible and is highly transparent and impermeable. Graphene also exhibits promising chemical characteristics, including a high chemical stability, high porosity and biocompatibility, and it is readily chemically functionalised through covalent and non-covalent modifications. These properties make graphene an exciting material that could revolutionise many technology and industry sectors.

A number of potential applications for graphene have already been identified, including in aerospace composites and coatings, semiconductor nanoelectronics, flexible batteries, flexible electronics, touch screens, transparent conductive films, solar cells, fuel cells, electromagnetic interference shielding, and radiation sensors.

Promising chemical applications that are currently being pursued include hydrogen storage, nano-sensors, desalination of seawater, separation of carbon dioxide and nitrogen gases, toxic material removal devices, and chemical catalysis. In addition, the biofunctionalisation of graphene with biomolecules (such as proteins, peptides, and DNA bases) may pave the way for new biotechnology applications. These applications are at different stages of realisation, and it is difficult to predict which ones will have a broad industrial and technological impact.

Nevertheless, graphene research is already attracting massive investments from universities, industry and governments. For example, last year, the European Commission pledged a sum of €1 billion for the fabrication of graphene and investigation into its potential applications. This initiative involves more than 140 academic and

commercial institutions in 23 countries. In addition, large companies like Apple, Intel and Samsung are looking into the use of graphene-based products in their future devices.

Computational chemistry is a branch of chemistry that uses computer simulation to solve chemical problems. With the advent of quantum chemical methods and high-performance computing facilities, computational chemistry provides a powerful means for exploring currently unknown chemistry and for designing efficient catalysts and other active molecules.

In my computational chemistry lab at the University of Western Australia, we are using sophisticated quantum chemical simulations to investigate potential applications of single-layer graphene sheets in chemical catalysis. Our research combines Australia's strength in three key areas: theoretical chemistry, experimental nano-chemistry, and the powerful supercomputer facilities located at the National Computational Infrastructure (NCI) facility in Canberra. We seek to address challenges in graphene catalysis that are of both fundamental and practical importance.

> *One such type of reaction is the inversion of non-planar aromatic compounds, such as fragments of the famous C_{60} carbon 'buckyball'*

In recent breakthrough research, we found that nano-sized fragments of graphene (so-called graphene nanoflakes) can significantly speed up the rate of a range of chemical reactions. One such type of reaction is the inversion of non-planar aromatic compounds, such as fragments of the famous C_{60} carbon 'buckyball'.

C_{60} is a highly symmetrical molecule that can be broken down into two basic fragments. These fragments are aromatic, bowl-shaped molecules that can convert from concave to convex structures. We have shown that graphene nanoflakes can efficiently catalyse this conversion through what we call π–π interactions. In addition, this work shows that the catalytic activity of graphene nanoflakes is not limited to bowl-to-bowl inversion reactions, but is extended to rotation and 'flip-flop' processes involving other non-planar aromatic compounds.

These findings are very exciting, because they demonstrate for the first time that graphene-like structures can efficiently catalyse chemical reactions via π–π interactions. Our longer-term goal is to further unravel the catalytic secrets of graphene and to progress towards industrial applications for graphene catalysts.

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