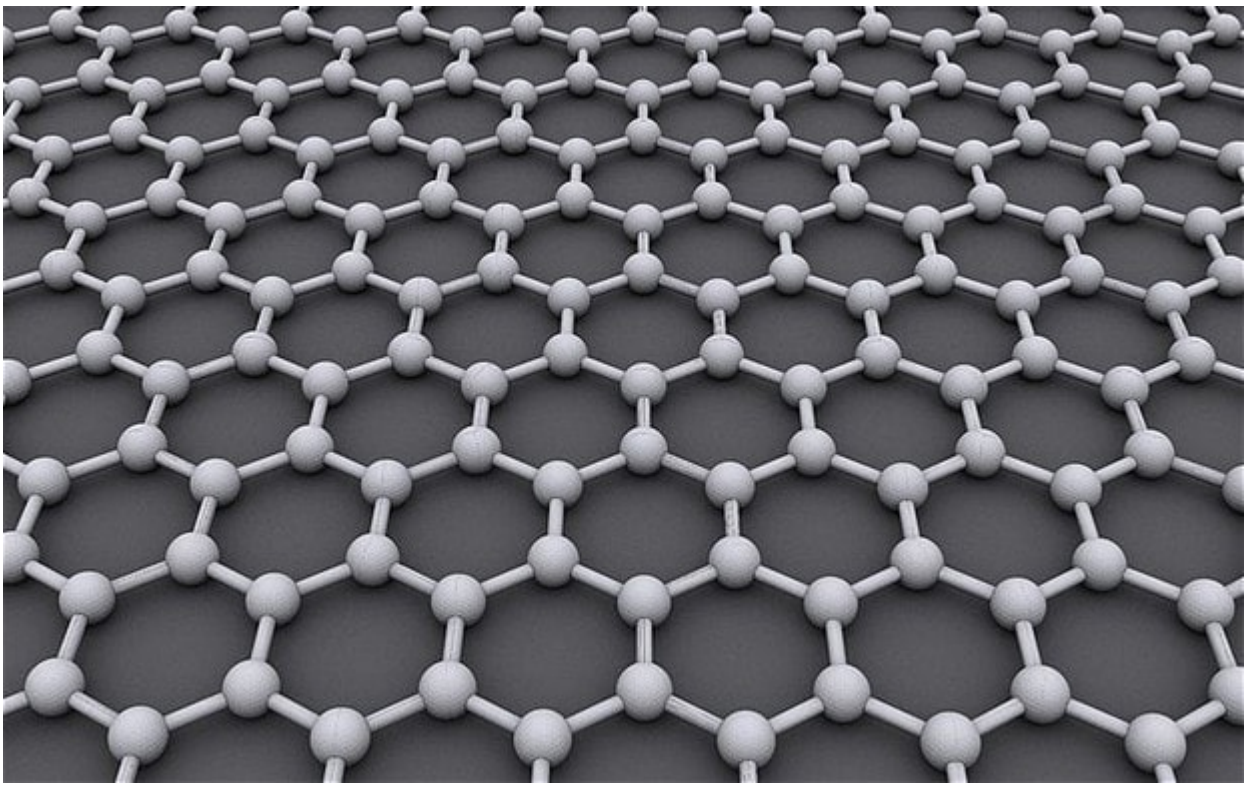
New 'Virtual Laboratory' will change how we approach material chemistry

UCL scientists have constructed a computer model that predicts the useful, physical properties of clay composites from their atomic make-up. Roger Highfield discusses the pratical applications of this advance



The ideal crystalline structure of graphene is a hexagonal grid Photo: Alexander Aius/Wikimedia Commons

By Roger Highfield

9:53AM GMT 16 Dec 2014

When the great theoretician Paul Dirac claimed in 1929 that the mathematical theory of the whole of chemistry is “completely known”, it seemed inevitable that chemists would soon abandon their test tubes and simply calculate how substances would behave using our most successful theory of all, quantum mechanics.

But although Dirac was the UK’s answer to Einstein, and won the Nobel Prize for predicting the existence of antimatter, it soon emerged that his vision, though correct in principle, was deeply impractical.

Last week, however, a team of chemists in University College London led by Prof Peter

Coveney **reported in the journal Advanced Materials** that it had taken a major step towards realising Dirac's dream of being able to work out the properties of a substance based on its atomic and molecular properties.

They have created a "virtual laboratory" in which it is possible to compute the properties of complex materials based on knowledge of their molecular structure and processing conditions. This advance, they believe, will pave the way towards a new materials revolution.

The difficulty with Dirac's original vision boils down to the size of a meaningful quantum calculation, which is astronomical. When mixing two substances together to trigger a reaction, chemists typically blend of the order of 1,000,000,000,000,000,000,000,000 molecules, give or take a few. Then they have to chart out what happens down to a timescale of a thousandth of a billionth of a second (a femtosecond).

"One would have to do the calculations in such tiny steps (less than a femtosecond) that you'd have to perform a gazillion (more than 10 billion steps) to get the system into the microsecond regime, which is just about relevant to real world chemistry," explains Prof Coveney. It would take years to carry them all out. "No one is going to give you a supercomputer for that long," says Prof Coveney. "And, besides, supercomputers are getting fatter, not faster, in that they can model larger slabs of matter, but for less time."

This has a surprising implication: we can't even convincingly work out how the boiling point of water and other basic properties emerge from the behaviour of its myriad molecules, viewed quantum mechanically.

Trial and error has been the order of the day. Walk around the Challenge of Materials gallery in the Science Museum and you will see the results of generations of experiments to figure out the link between a chemical recipe and desirable properties, from Egyptian glass to Thomas Heatherwick's first public commission: Materials House, a sculpture consisting of 213 layers of materials from Astroturf to Segovia lace.

The history of materials such as carbon-fibre-based materials, light-emitting diodes and high temperature superconductors teaches us that it can take decades from the discovery of a new material to honing it for real world applications.

Now Prof Peter Coveney, James Suter and Derek Groen have shown that it is possible to calculate the properties of a material from the bottom up, using supercomputers in the UK

and Germany to extrapolate from the quantum domain where, in effect, all chemistry boils down to the behaviour of electrons, to slabs of material many microns in extent, comprising of millions of atoms.

They focused on composites of clays and polymers. Since the late Eighties, clays have been combined with synthetic polymers (such as nylon) to produce composites with superior properties such as enhanced strength for use in cars, aircraft and elsewhere.

At the atomic level, clay minerals consist of stacks of thin aluminosilicate sheets, based on aluminium, silicon, and oxygen atoms, separated by a few billionths of a metre. The sheets are about one micron across, stacked like a disordered pack of cards, with between a few sheets and one thousand in any single pile. The trick is to use a polymer to coax the sheets to organise in particular ways, a feat nature manages with ease in materials such as shell, bone and mother of pearl.

Prof Coveney's team found a way to simulate the properties of these composites, starting with their component electrons (to capture the way the polymer interacts with clay) through the movement of their atoms to the behaviour of millions of atoms. They compared characteristics of the virtual nanocomposites they synthesised in their virtual lab with the real thing and found they were reassuringly similar.

This feat is of profound interest because the problem of straddling different levels of understanding is common in science: we can see chemicals at work in the brain, map nerve connections and measure large scale flows of blood that take place during thinking but bridging these descriptions is tough.

When it comes to practical implications, this advance will speed the development of wonder materials. Take graphene, a two dimensional form of carbon, for example. The material shows so much promise in so many ways that an exhibition about it is already being planned at the Museum of Science and Industry in Manchester, where the great graphene pioneers and Nobellists Andre Geim and Kostya Novoselov work nearby in the university.

Prof Coveney believes computer modelling will speed the applications of graphene: "At the UK National Graphene Institute in Manchester, a colleague is already working on using graphene in enhanced performance condoms." The possibilities range far beyond graphene, of course. It is also possible to envisage a day where a 3D printer can not only print out the right shape but also customise a material with designer properties for a given application.

When that becomes routine, Dirac's dream will have become a reality.

Roger Highfield is the director of external affairs, Science Museum