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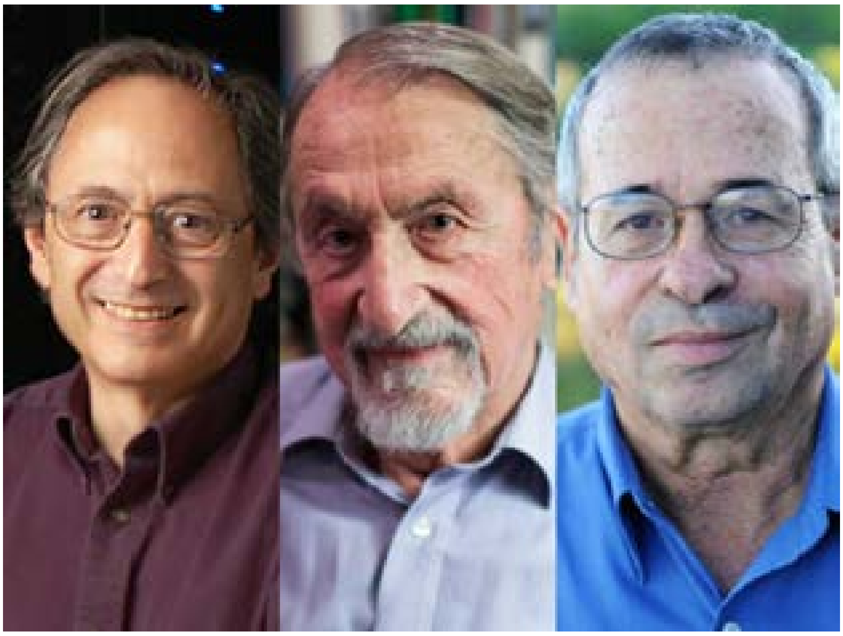
Award winning models

The Nobel Prize is the most prestigious prize in science. A chemistry prize is awarded each year and in 2013 it was awarded to Martin Karplus, Michael Levitt and Arieh Warshel whose work allowed the development of complex computer models of compounds and reactions. Why was this so significant?



The winners of the Nobel Prize for Chemistry 2013: Michael Levitt, Martin Karplus and Arieh Warshel

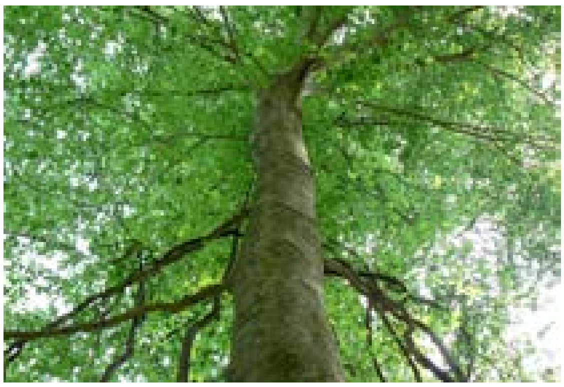
Chemists work with a huge variety of substances; some are elements, others are compounds. Most of the compounds which you encounter in school are relatively simple: carbon dioxide, for instance, contains 2 atoms of oxygen bound to a carbon atom. You might use some bigger molecules like glucose, $C_6H_{12}O_6$, or starch. As the molecules get bigger it becomes harder to visualise exactly what is going on when they react.

Many molecules which have important functions are very big. Protein molecules, for instance can contain thousands or even tens of thousands of atoms bound together in complex shapes. It can be important to understand how reactions in these huge molecules take place – for example how a drug binds to an active site. This enables drug development to become more efficient and therefore cheaper.

Another complex reaction is that of carbon dioxide and water in chlorophyll. This is the photosynthesis reaction and it forms glucose and oxygen using energy from the sun to power the reaction. The equation for the reaction itself looks complex enough:

$$6CO_2 + 6\,H_2O \rightarrow C_6H_{12}O_6 + 6O_2$$

But useful though this equation is, it does not give any information about how the electrons are moving within the molecules to allow this transformation to take place. It also does not show how the chlorophyll catalyst is involved – where the various molecules bind to the chlorophyll and how the electrons move from one atom to another.



Every green leaf contains chloroplasts, each of which contains the chlorophyll needed for photosynthesis to produce glucose and oxygen.

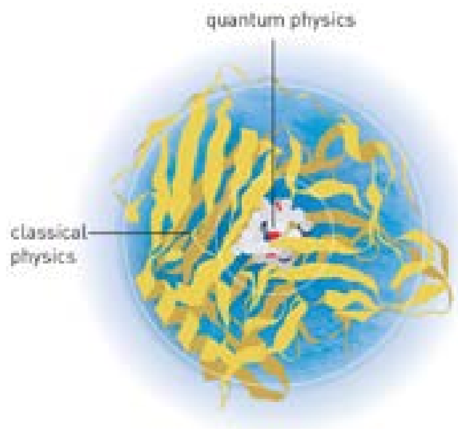
Without this information it is very difficult to design an artificial catalyst which will do the same job – and if a good artificial catalyst were developed, it would help to solve both the need for cheap, renewable energy and also the increase in the carbon dioxide concentration in the atmosphere.

The chlorophyll molecule which is the key to this is very complex. The key part of the molecule is the reaction centre which is where the water molecules are split apart. For all the huge size of chlorophyll, the reaction centre is relatively small, containing only a handful of atoms.

The 2013 Nobel Prize for chemistry has been awarded to three chemists whose work has allowed significant progress in understanding this reaction and many other reactions. They are not the ones who have solved the structure or worked out what the reaction pathway is, but they have given others the tools to aid their understanding of large molecules.

According to the Nobel Prize committee, the prize has been awarded for 'the development of multi-scale models for complex chemical systems.' What the three prize winners have done is to lay the foundations for powerful programmes which are used to understand and predict chemical processes.

You may have used a variety of models in school to help you understand the structure of various chemicals. Many of these are 'ball and stick' models where ball shapes for atoms are held together with stick pieces. These have their uses but are limited when it comes to understanding huge molecules – or even how electrons move in small molecules.



A pixelated image can be understandable if the most important part is in focus. The breakthrough for which the Nobel Prize was awarded was the realisation that the most detailed calculations of a molecule can be carried out just on the most important part of it.

A space-filling of a chlorophyll molecule. Black balls are carbon atoms, white is hydrogen, red is oxygen, turquoise is nitrogen, and orange is magnesium.

Computer models are faster and more powerful. But there is a problem. There are two sets of equations which can be used to predict how chemicals will react. One set are based on Newton's classical physics. These equations were established by Sir Isaac Newton who lived from 1643 to 1727. They are relatively simple and do not take too much computing power, allow the modelling of large molecules, but not the modelling of chemical reactions. The other equations were developed in the 20th century, are far more complex, but do allow reactions to be modelled. These are called quantum mechanics. As far more computer power is needed for quantum mechanics only small molecules can be modelled using them.

What Karplus, Levitt and Warshel managed to do was to make the two sets of equations work together. They realised that for large molecules, they could use Newtonian equations to model most of the molecule and quantum mechanics to model the reaction centre. This is similar to having most of a picture made of large pixels but the important part, the face, in far more detail. This was a revolutionary break-through and has provided chemists with powerful models to help them simulate complex reactions.

Vicky Wong is chemistry editor of Catalyst.

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