Tying molecules in knots

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A new generation of lighter, stronger plastics could be produced using an intricate chemical process devised by scientists.

Chemists working on the nanoscale – 80,000 times smaller than a hair's breadth – have managed to tie molecules into complex knots that could give materials exceptional versatility.

By weaving threads of atoms into the shape of five-point stars, researchers at the University of Edinburgh have created the building blocks of materials that could be supremely flexible and shock absorbent.

They hope that the new molecules – known as pentafoil knots – will mimic the characteristics of complex knots found in proteins and DNA, which help to make some substances elastic.

In natural rubber, for example, 85 per cent of its elasticity is caused by knot-like entanglements in its molecule chain.

Creating knotted structures in the laboratory should make it easier for scientists to observe and understand exactly how entanglements influence a material's properties.

And being able to produce materials with a specific number of well-defined knots, rather than the random mixture that occurs in today's plastics and polymers, scientists could exercise greater control when designing materials.

The research, funded by the Engineering and Physical Sciences Research Council, is reported in *Nature Chemistry* journal.

The Edinburgh team, working with researchers from the University of Jyväskylä in Finland, is the first to create a knot with five crossing points.

The pentafoil, also known as a Solomon's seal knot, has symbolic significance in many cultures and is the central emblem on the flags of Morocco and Ethiopia.

Deliberately tying molecules into knots so that its properties can be studied is extremely difficult. Until now, only the simplest type of knot – the trefoil, with three crossing points – has been created by scientists.

Remarkably, the thread of atoms that the Edinburgh team has tied into a five-star knot is just 160 atoms in length and measures a 16-millionth of a millimetre.

Using a technique known as self-assembly, the researchers produced a chemical reaction in which atoms were chemically programmed to spontaneously wrap themselves up into the desired knot.

Principal researcher David Leigh, Forbes Professor of Organic Chemistry at the University of Edinburgh, said: "It's very early to say for sure, but the type of mechanical cross-linking we have just carried out could lead to very light but strong materials - something akin to a molecular chain mail.

"It could also produce materials with exceptional elastic or shock-absorbing properties because molecular knots and entanglements are intimately associated with those characteristics. By understanding better how those structures work - and being able to create them to order - we should be able to design materials that exploit those architectures with greater effect."

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Link to the rotating pentafoil knot: users.jyu.fi/~krissane/Knot.html

Provided by University of Edinburgh