Research findings could revolutionise industrial catalysts

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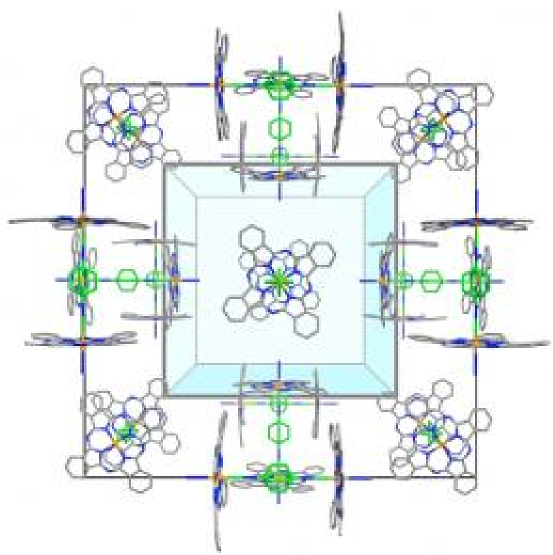

The crystal structure of the nanoporous crystal showing the "molecular wall-tie" ligands (green) binding between the iron centres.

(PhysOrg.com) -- It is a long-held ambition of scientists to prepare porous solids within which they are able to mimic the sophisticated chemistry performed by nature. Research published today (26th March 2010) in the journal *Science* describes how a group of scientists have made a breakthrough and are now a step closer to achieving this ambition.

Researchers from Cardiff University and the University of Manchester succeeded in engineering crystals that are able to maintain their structure, providing a permanent porous matrix within which chemical reactions can take place. With this new porous crystal, made from an iron-containing compound called phthalocyanine, the group are looking to nature to maximise its potential within the field of industrial catalysts.

They are taking their initiative from enzymes, nature's catalysts that have a wide range of roles in biological environments, including speeding up chemical reactions within the human body. They are particularly interested in hemoproteins, a type of protein that contains iron porphyrin, a close relative of iron phthalocyanine, that are unusual in the diversity of tasks they are able to perform. The group used the Science and Technology Facilities Council's (STFC) Daresbury Laboratory and Diamond's Single Crystal Diffraction beamline I19 to understand whether it is possible to make porous crystals with the reactivity of hemoproteins in order to produce more effective man-made catalysts.

Lead author on the paper, Prof. Neil McKeown from Cardiff University's School of Chemistry, explains the significance of the group's achievement: "Normally the voids within nanoporous crystals of this type need to be filled with organic solvent and if this is removed they simply collapse losing their porosity and therefore the space in which to carry out chemical reactions. But by taking inspiration from the use of cavity wall-ties in architectural engineering, we have stabilised our crystals with the addition of suitable ligands, that can bind simultaneously to two iron atoms, thus acting as 'molecular wall-ties."

The design of the new type of crystal is such that they can exist happily in water based environments and are accessible to gas molecules. This aspect makes them a contender for future industrial catalysts.

More information: Heme-Like Coordination Chemistry Within Nanoporous Molecular Crystals, C. Grazia Bezzu, Madeleine Helliwell,

John E. Warren, David R. Allan, Neil B. McKeown. *Science* 26 March 2010: Vol. 327. no. 5973, pp. 1627 - 1630.
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