

The whole procedure is iterative — solutions are repeatedly assessed, the lowest-energy models are clustered to identify common features and then further effort is concentrated on more variable regions. Rosetta also analyses peptide sequences found in analogous proteins from species of organisms other than that of the target sequence, as such proteins are expected to have similar three-dimensional structures to the target molecule. The whole process is terminated when conformations are identified that have significantly lower energies than the average energy of the protein.

The algorithms used in Rosetta are sophisticated, and the computing resources required to carry out the calculations, to keep track of results and to plan future strategies, are awesome. The authors therefore used a procedure called Rosetta@home⁶, which distributes the calculations across a network of home computers — more than 70,000 in June 2006 — whose owners allow the program access to their idle machines.

There is still much to be done. Cynics might mutter that one success doesn't prove that Qian and colleagues' method² is truly general, and

that it should be assessed further using known structures. Nevertheless, this approach demonstrates real progress in several respects: the use of enormous computational power; the exploitation of known three-dimensional structures; the development of powerful search algorithms that relate those structures to new sequences; and the steadily improving tactics used to determine low-energy conformations of molecules. The benefits will be seen in structure-based drug design and in improved models for crystallographic calculations. And in the future, this method might provide structural information about intractable molecules that are difficult to study experimentally. ■

Eleanor J. Dodson is at the York Structural Biology Laboratory, Department of Chemistry, University of York, Heslington, York YO10 5YW, UK. e-mail: e.dodson@ysbl.york.ac.uk

1. Sela, M., White, F. H. Jr & Anfinsen, C. B. *Science* **125**, 691–692 (1957).
2. Qian, B. *et al.* *Nature* **450**, 259–264 (2007).
3. Moulton, J. *Phil. Trans. R. Soc. Lond. B* **361**, 453–458 (2006).
4. <http://predictioncenter.org>
5. McCoy, A. J., Grosse-Kunstleve, R. W., Storoni, L. C. & Read, R. J. *Acta Crystallogr. D* **61**, 458–464 (2005).
6. Das, R. *et al.* *Proteins* doi:10.1002/prot.21636 (2007).

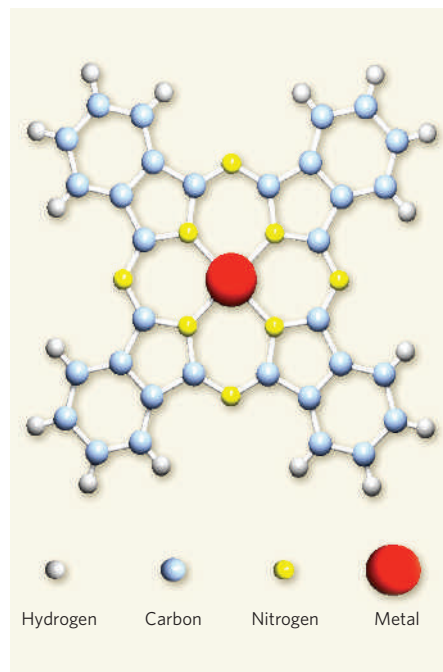


Figure 1 | Structure of metal phthalocyanines. Metal phthalocyanines are a class of molecule that comprises an organic, four-leaf-clover structure with a metal at the centre. Heutz *et al.*¹ show that the magnetic state of films of these molecules can be switched by controlling their crystalline structure.

MATERIALS SCIENCE

Magnetic blue

Jeroen van den Brink and Alberto F. Morpurgo

A commonly used blue dye is more than just a pretty colour. This material and its relatives are semiconductors, and their magnetic properties can be controlled by engineering their crystal structure.

Organic compounds are rarely magnetic, but metal phthalocyanine (MPc) materials are notable exceptions to this rule. Reporting in *Advanced Materials*, Heutz *et al.*¹ now show that the magnetism of MPcs can be controlled. By changing the crystal structure of an MPc film, the authors switched the material from being in a magnetically ordered state to a non-magnetic one. This approach might provide a method for customizing the magnetism of molecular materials.

MPcs are flat molecules that take the shape of a four-leaf clover. They consist of an outer ring, formed from nitrogen, carbon and hydrogen atoms, with a metal atom bound at the centre (Fig. 1). The first molecule of this class was discovered at the beginning of the twentieth century, and had a copper atom in the middle. Because of its brilliant blue colour, the compound was immediately seized upon for use in paints and dyes. The hue also inspired the name 'phthalocyanine', which was taken from the Greek-derived words for rock oil (naphtha) and blue (cyan).

Since then, more than 70 MPcs have been synthesized, each with a different central atom or group of atoms. The properties of these

compounds vary widely. For example, simply attaching chlorine atoms to the aromatic rings in copper phthalocyanine (CuPc) modifies the electronic absorption spectrum of the molecules. This process is used to add subtle green tones to blue paint. No great conceptual leap is required to see that similar structural modifications to MPcs could result in compounds with other interesting properties.

In fact, chemists have long known how versatile MPcs can be. Apart from their common use as dyes in the textile and paper industry, they can also act as catalysts, and they have even been investigated as anticancer agents. But perhaps their most interesting characteristics are their magnetic and electronic properties. If a transition-metal atom is placed in the centre of the ring, MPcs carry a magnetic moment because of the particle spin of the transition-metal atom. The spin value varies depending on the metal used, so that MPcs can be thought of as nanomagnets, the magnetic strength of which can be controlled at a molecular level.

Physicists are only just starting to explore systematically the full potential of MPc-based compounds. The leitmotif of this work is the addition of electrons to the materials to probe

changes in their electrical and magnetic properties. Of particular interest is the unexpectedly large number of electrons that can be hosted by MPcs — up to four or five on a single molecule. The resulting charge density can be tuned by adding electron-donating atoms (such as lithium, potassium or rubidium) to the materials. This 'electron-doping' technique has also been used on buckminsterfullerene (C₆₀), the famous football-shaped carbon molecule that has been a fertile playground for condensed-matter physicists for almost two decades.

The latest experiments on MPcs have produced some surprises. These compounds are usually semiconductors, but several MPc films turn into metallic conductors when electron-doped with potassium atoms². The variation of conductance with the amount of potassium incorporated into the films provides information about which molecular orbitals the donated electrons occupy in each MPc (ref. 3). Other experiments reveal that the magnetic properties of manganese-containing MPcs can be tuned by varying the concentration of lithium dopants⁴.

The big idea behind all this work is that it should be possible to engineer the electronic properties of solids by chemical actions at a molecular level. This proposal is certainly not new. But researchers who have attempted this in the past have almost invariably been confronted with a harsh reality: small molecular modifications made to tune the bulk electronic properties of a solid often cause drastic changes to the packing of the molecules in that solid. Such changes to the crystal packing cannot usually

be controlled, and can easily eclipse any chemically induced changes to the electronic properties. In most cases, this has prevented systematic progress. MPCs, however, are different from other compounds; in most MPC crystals, the molecules are packed in a similar way, so that structural effects are less likely to be a problem.

Heutz *et al.*¹ now show that not only do the crystal structures of MPCs create fewer problems, but they may also be turned to advantage. The authors controlled the crystal form of thin MPC films by growing them on different substrates; this allowed them to exploit the fact that the interaction between the magnetic moments of neighbouring molecules depends on the relative orientation of those molecules. On one of the substrates, the orientation of the molecules in the film is such that the interaction between magnetic moments vanishes. In this case, the MPC nanomagnets point in random directions and do not create a net magnetic moment. But on a different substrate, the molecules were slightly rotated with respect to their previous orientation. This is enough to switch on the magnetic interaction between the molecules. In other words, the authors engineered the macroscopic ordering of the nanomagnets by controlling the crystal form of the material.

The authors' findings¹ are the latest in a growing body of work that explores the unique properties of MPCs. It is now clear that these compounds display a rich interplay of electronic, magnetic and structural properties, with potential technological relevance. Stimulated by this experimental activity, theorists have also started to investigate electron-doped MPCs, and have made some startling predictions. For example, they propose that, under appropriate conditions, these systems may become superconductors at high temperatures⁵, adding to the already impressive roll-call of MPC properties.

It is always difficult to predict how any field of research will develop. But it is clear that multifunctional MPCs are potential building-blocks for future materials. We would not be surprised if physicists soon start to approach their colleagues in chemistry and materials-science departments asking for a greater variety of well-characterized MPC compounds. At present, MPC materials may just be the toys of blue-skies researchers. But once they make it out of the playground, they could become invaluable. ■

Jeroen van den Brink is at the Instituut-Lorentz for Theoretical Physics, Leiden University, Postbus 9506, 2300 RA Leiden, the Netherlands. Alberto F. Morpurgo is at the Kavli Institute of Nanoscience, Delft University of Technology, Postbus 5, 2600 AA Delft, the Netherlands. e-mails: brink@ilorentz.org; a.morpurgo@tnw.tudelft.nl

1. Heutz, S. *et al.* *Adv. Mater.* doi:10.1002/adma.200701458 (2007).
2. Craciun, M. F. *et al.* *Adv. Mater.* **18**, 320–324 (2006).
3. Craciun, M. F., Rogge, S. & Morpurgo, A. F. *J. Am. Chem. Soc.* **127**, 12210–12211 (2005).
4. Taguchi, Y. *et al.* *J. Am. Chem. Soc.* **128**, 3313–3323 (2006).
5. Tosatti, E., Fabrizio, M., Tóbiš, J. & Santoro, G. E. *Phys. Rev. Lett.* **93**, 117002 (2004).

PLANETARY SCIENCE

A twist on periodicity at Saturn

Margaret Galland Kivelson

Saturn's nominal rotation period is timed by a 'radio clock' that counts bursts of emissions controlled by the planet's magnetic field. Buffeting by the solar wind may explain the clock's irregularities.

Einstein showed us that measurements of time made in systems moving at different speeds will not agree. What would he have thought of a clock whose ticking depends on how fast the solar wind — a gas of charged particles, or plasma, constantly flowing outwards from the Sun — is blowing? Yet that is what, on page 265 of this issue, Zarka and colleagues¹ tell us is the case for the radio-emission clock that has been used to infer Saturn's rotation period.

Time-keeping on planets is linked to their orbital periods ('years') and their rotation periods ('days'). Strangely, it is not straightforward to determine the rotation periods of the gas-giant planets: Jupiter, Saturn, Neptune and Uranus. These planets lack solid surfaces with features to track as the planet rotates. Images of the gas giants allow one to track clouds, but their motions are not precisely tied to the rotation of the interior. How, then, do we establish rotation rates?

A particularly fruitful approach has been to monitor the intensity of radio-frequency

emissions from sources close to the planet. Such emissions arise in a planet's magnetosphere, the region of space dominated by its magnetic field (Fig. 1), and their intensity depends on the angle between the observer and the magnetic field at the source. If the planet's internally generated magnetic field is asymmetric about its spin axis, the direction of the field at the source will seem to nod up and down as the planet spins, and the intensity of the observed emissions will vary with the rotation period. The planetary rotation rates of Jupiter², Neptune and Uranus have been identified in this way.

Saturn emits radio signals modulated at a period of about 10.75 hours. This period has been used to define the period of rotation of the interior³, but it has proved hard to understand why the radio power varies periodically because the best available measurements fail to detect any asymmetry of the internal magnetic field⁴. Possibly even more puzzling is the recognition that the period of the modulation is not fixed. The first hints of that, initially greeted

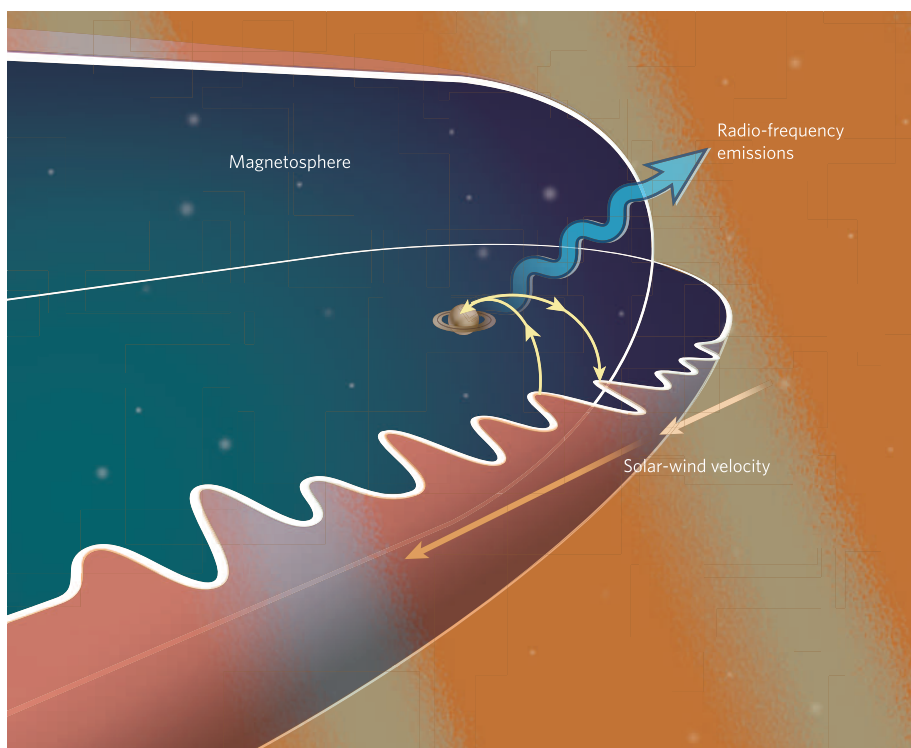


Figure 1 | Generation of radio emissions at Saturn. Saturn's magnetosphere is embedded in the solar wind, here shown as flowing away from the Sun at speeds that increase and decrease periodically (the faster-flowing portions are depicted in dark orange). Radio emissions are produced where electrical current flows into Saturn's auroral ionosphere. Zarka *et al.*¹ show that the power of the radio emissions is modulated periodically, and that the period varies with the speed of the solar wind, possibly because the currents are generated by wave-like disturbances at shifting locations along the magnetospheric boundary.