

alkenes to epoxides<sup>7</sup>, which is an important reaction in synthetic organic chemistry and chemical technology. The porphyrins adhere to the gold surface, which serves two important functions — it holds the molecules in place, enabling them to be scanned and imaged with the STM tip, and also activates them for catalytic function. Here, the porphyrin catalyst binds an oxygen atom at its metal centre (by breaking apart molecular oxygen, O<sub>2</sub>) and then transfers it to an alkene to form an epoxide (Fig. 1). Following this step, the porphyrin is free to bind another oxygen atom and take part in a second catalytic cycle and so on.

The breakthrough in Elemans' study is the ability to capture high-resolution snapshots of these events at the single-molecule level. Because these snapshots view individual porphyrin molecules, they offer new molecular-level insights concerning the mechanism of this reaction. In this case, after the gold-bound porphyrins were exposed to molecular oxygen, those that reacted to form catalytic centres by binding an oxygen atom could be directly recognized as clear bright spots in the STM image. The distribution of the catalyst centres could therefore be mapped, and, through a statistical analysis of the images, it was deduced that oxygen-binding molecules preferentially sit next to each other. From this placement, it was concluded that one molecule of O<sub>2</sub> 'feeds' two neighbouring porphyrin molecules.

After mapping the distribution of the 'bright' oxygen-binding catalyst molecules, the catalytic reaction was allowed to run *in situ* by introducing alkene molecules. As the alkenes are transformed into epoxides, the manganese porphyrins give up their oxygen atoms and the density of bright spots (corresponding to oxygen-binding catalyst molecules) in the STM image decreased, confirming that the catalytic reaction had progressed. The epoxide products could be detected in the gas phase above the solution by gas chromatography. Additionally, in the absence of a chemical reaction (that is, no added alkene) it was shown that the number of oxygen-containing catalyst molecules could be maintained at a constant level, attesting to the long-term stability of this immobilized catalyst.

The ability to image single catalyst molecules 'at work' offers insights that would not have been possible with conventional ensemble techniques that average over many molecules. Notably, the fate of single oxygen molecules — which distribute themselves as two oxygen atoms to two neighbouring catalysts — has been clarified. How this happens when the metal centres in neighbouring molecules are such a large distance apart (~20 Å) will be a matter for further study. A next step could be to image the reactions of the catalyst with O<sub>2</sub> and with the alkene using video-rate STM. This should enable a more detailed temporal picture of

the evolution of the catalytic process to be built up.

It is clearly exciting that catalytic reactions on surfaces can be imaged under ambient laboratory conditions. However, in order to follow them in real time with STM, the rate and turnover of the reactions has to tally with the maximum rate at which images can be acquired. This consideration is likely to limit the number of ambient reactions that can be meaningfully studied with this technique, at least at this stage. Nevertheless, there are other reactions that can be explored, such as those important in fuel cells, which includes the reduction of molecular oxygen to water using metal-organic complexes. Such reactions are very much in the limelight as scientists are trying to develop new catalysts and understand their mechanism of operation.

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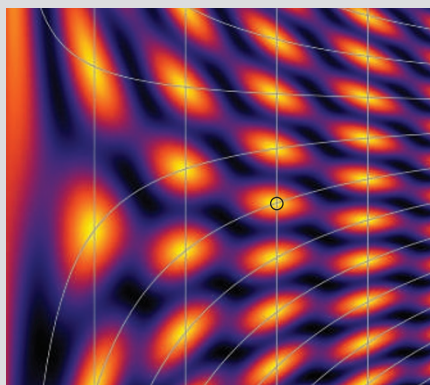
## QUANTUM INFORMATION

### High fidelity

Quantum computers are expected to perform much faster than classical computers because they exploit the ability of quantum bits to exist in a superposition of different states. A classical bit can only ever take on a value of '0' or '1', but a quantum bit or 'qubit' can have any combination of these two values. However, real-world qubits must satisfy stringent requirements to take these ideas from the blackboard to the motherboard.

Daniel Loss, a theoretical physicist from the University of Basel in Switzerland, has been exploring the performance of different types of qubits for a number of years. Now, on page 312 of this issue, Loss and colleagues in Basel and the University of Valencia in Spain suggest that qubits based on molecular magnets could have advantages over other approaches (*Nature Nanotech.* **2**, 312–317; 2007).

They study a polyoxometalate molecule in which two vanadium oxide (VO)<sup>2+</sup> groups



are separated by a core of molybdenum oxide. Each (VO)<sup>2+</sup> group has an electron spin that can point up or down, or in a superposition of both directions, so the molecule plays host to two spin qubits, with the interaction between them depending on the number of electrons on the core. The spins do not interact with each other when

there are an even number of electrons on the core, but if an electron tunnels on or off the core, leaving an odd number, they will start to interact.

The length of time over which the interaction, or 'gate', is turned on determines the final state of the spins. This graph shows how a figure of merit known as the gate fidelity is predicted to vary as a function of time (x axis) and the strength of the interaction between the spins (y axis). The maxima are indicated in yellow, with the circle indicating the highest calculated fidelity of 0.99.

The calculations were performed for a single molecule with electrons tunnelling from the core to a scanning probe tip and back, but Loss and co-workers believe that their system could be scaled to large numbers of qubits by combining molecular self-assembly techniques with a crossbar electrode geometry.

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