complex operation. Our retinas do it routinely, as do algorithms in some image-processing software; genetically engineered bacteria and DNA networks have also been devised to carry out this operation. Now, A. Prasanna de Silva and co-workers from Queen's University, Belfast, have performed this task using a filter paper soaked in a solution of three molecules — a pH sensor, a photo-acid generator, and a pH buffer — and a UV lamp.

The researchers chose a pH sensor known to fluoresce under irradiation in the presence of a photo-acid generator (triphenylsulfonium chloride) — showing behaviour known as 'off–on–off' fluorescence. The sensor molecule comprises an aromatic core, the fluorescence of which is quenched intramolecularly by an amino nitrogen lone-pair. Under irradiation, photolysis of the triphenylsulfonium chloride generates a proton and a photoproduct, 2-phenylthio-biphenyl. These two species go on to trigger changes in the pH sensor's fluorescence. First, protonation of the sensor's amine moiety halts the intramolecular quenching mechanism, turning the fluorescence on, but the photoproduct accumulates as the irradiation continues, and the fluorescence is quenched by another mechanism: photo-induced electron transfer from the photoproduct. Thus, an area irradiated — through a mask to create a pattern — first becomes bright then dark again. What leads to the visualization of the edge of the pattern is that the photo-generated protons diffuse away from of the irradiated area. When the protons reach the non-irradiated area, within which the photoproduct quencher has not yet sufficiently accumulated, fluorescence is turned on.

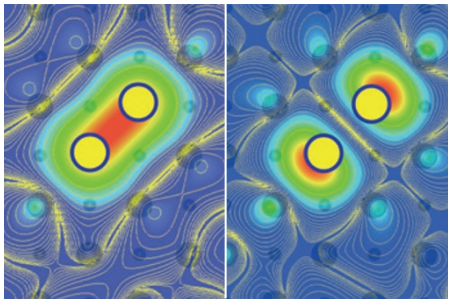
The researchers ensured only the edge of the pattern would become bright by adjusting the pH (using a sodium carbonate buffer) and the wetness of the filter paper so that the protons turn on the fluorescence in only a limited area (1–2 mm wide) outside the irradiated pattern. Similar edge visualization was achieved with two other off–on–off pH sensors, demonstrating the generality of this molecular logic-based computation step. *AP*

THEORETICAL CHEMISTRY

Electrides explained

J. Am. Chem. Soc. **137,** 3631–3637 (2015)

Electrides are something of a chemical curiosity. They are ionic materials within which electrons act as anions and they find roles in catalysis and as reducing agents in organic synthesis. They have been shown, both theoretically and experimentally, to exist in several materials at high pressures. One theoretical framework for high-pressure electrides, put forward by Mao-sheng Miao at California State University and Roald Hoffmann at Cornell University, argues that the interstitial spaces in an elemental or ionic lattice feature quantized energy levels analogous to those of atomic orbitals. With increasing pressure, the respective energy levels of atoms on lattice sites and of interstitial spaces change, and electrides form when the energy of the interstitial space is less than that of the valence orbital of the lattice site atoms. The electrons that then occupy those spaces have been dubbed interstitial quasiatoms (ISQs).



AMERICAN CHEMICAL SOCIETY

Now, Miao and Hoffmann have carried out theoretical studies on a number of materials at high pressures to examine the behaviour of ISQs and compare them with 'real' atoms and molecules. By calculating electron density in double hexagonal close-packed sodium and hexagonal magnesium, at 300 and 800 GPa respectively, they show that ISQs can behave analogously to anions — for instance, the sodium high-pressure electride carries a charge in the interstitial spaces very close to that on the sulfur atoms in Na_2S at high pressure. They can also interact with each other by forming metal-like bonding: the model for the magnesium high-pressure electride shows planes of delocalized electron density.

Having noted these similarities to conventional bonding, they also carried out calculations on a 'compression chamber' made up of 108 helium atoms in a face-centred cubic geometry. When two electrons are added to the system, features that bear striking resemblance to a conventional HOMO and LUMO are seen in the calculated electron-density maps (pictured). Similar features were also seen when ISQs were located adjacent to Li or Mg dopants in the same lattice, suggesting that interstitial quasiatoms could effectively form so-called quasimolecules. *CH*

Written by Enda Bergin, Stephen Davey, Claire Hansell and Anne Pichon.

blogroll

Comment etiquette

Post-publication peer review is a reality, so what should the rules be?

Scientific discussions about published papers, which used to take place in lab meetings or over coffee at conferences, now also happen on blogs (especially in their comment sections), discussion boards and Twitter. Websites such as PubPeer and BioMed Central host or aggregate these discussions, but the standards and etiquette of modern post-publication peer review remain to be codified.

One question is that of anonymity. As Dave Fernig discusses at Ferniglab Blog (http://go.nature.com/wKRik2), anonymous comments are typically associated with negativity, rather than constructive engagement. Nevertheless, Fernig argues the case for anonymity, stating that without it the academics with the least power (for example, early-career researchers) would not be able to speak their mind.

However, allowing anonymity or failing to verify identities can lead to dirty tactics. Julian Stirling shares on PhysicsFocus (http://go.nature.com/TTe8kw) his first-hand experience of identity theft and sock-puppetry (multiple accounts used by a single person) from comments on his recent paper in *PLoS ONE*. This question of anonymity in post-publication peer review also has legal ramifications. Alison McCook, at Retraction Watch (http://go.nature.com/qUMpxD), reports that PubPeer was allowed by a US Circuit Court judge in Wayne County, Michigan to protect the anonymity of its commenters in relation to a lawsuit brought by a scientist aggrieved at the treatment of his papers on the site.

Finally, Philip Moriarty experimented, at the Winnower (http://go.nature.com/qnW3Lt), with post-proposal peer review, posting online for discussion a freshly submitted grant proposal to the UK's EPSRC (http://go.nature.com/7OLmtF). So far, the concept has attracted more comments than the proposal itself. Maybe this was fated, being the first of its kind?

Written by François-Xavier Coudert, who blogs at http://blog.coudert.name and tweets as @fxcoudert