The high reactivity of {001} facets also suggests that the crystals synthesized by Lu *et al.*[3] may exhibit higher photocatalytic efficiency in comparison with currently used TiO_2 photocatalysts. Since the report of Fujishima and Honda in 1972[11], TiO_2 has become the most widely used semiconductor in photocatalysis, and research aimed at enhancing its efficiency has intensified over the years[12]. In particular, due to the anatase (001) surface's ability to dissociatively adsorb water, these crystals could be promising photocatalysts for the splitting of water in H_2 and O_2 (ref. 13). In photocatalysis, electrons and holes generated in the TiO_2 crystal by absorption of UV photons can diffuse to the surface, where they can be transferred to adsorbed species causing their reduction and oxidation, respectively. The microscopic details of these electron-transfer processes are not yet well understood, but the transfer is expected to be more efficient if the adsorbate and the surface are strongly coupled, as when adsorbed species are dissociated.

To use Lu and colleagues' crystals for photocatalysis or any other application, however, the fluorine atoms terminating/passivating the different surfaces must first be removed. They report[3] that a simple heat treatment is sufficient to clean the surfaces, without altering the crystal structure and morphology. As previously mentioned, however, the clean anatase (001) surface reconstructs under UHV conditions[8]. The reconstruction strongly stabilizes the surface[14] and at the same time largely reduces its reactivity: calculations indicate that the fraction of active sites for water dissociation is reduced by a factor ~0.25 with respect to the unreconstructed surface (X. Q. Gong and A. Selloni, unpublished work). The question remains whether, in an aqueous environment, fluorine atoms can be replaced by water or other functional moieties, such as photosensitizer molecules, before the surface reconstructs and thus becomes much less reactive. Regardless, the paper by Lu and co-workers still provides clever and useful hints on how a combined approach based on computer simulation and surface chemistry can be used to engineer the properties of metal oxide crystals.

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MATERIAL WITNESS

Renewing old promises

One of the curious aspects of a new prediction that hydrogen can be a high-temperature superconductor under pressure[1] is that the same conclusion was voiced in the same journal forty years ago. In 1968, Neil Ashcroft at Cornell University argued[2] that the conventional description of superconductivity in terms of the pairing of electrons mediated by phonon lattice vibrations — the so-called BCS picture of John Bardeen, Leon Cooper and Robert Schrieffer — made solid hydrogen a good candidate for a superconductor with an unprecedentedly high transition temperature (T_c).

Ashcroft pointed out that the lightness of hydrogen atoms gives the solid a high phonon frequency, and that the lack of core electrons in hydrogen promotes strong coupling between electrons and phonons; both factors favour a high T_c. He held back from making explicit predictions of T_c (which would be pressure-dependent) although one can deduce that his lower limit was about 50 K. Ashcroft proposed that Jupiter might have a hydrogen-rich interior warm and dense enough for part of it to be superconducting.

This story can be traced back still further to the original notion that hydrogen might be metallic. That idea is normally thought to originate with Eugene Wigner and his colleague Hillard Huntington[3], although they attributed the notion that many substances should become metallic under pressure to the crystallographer J. Desmond Bernal, a protégé of William Bragg. This prediction wasn't verified until 1996, using shock compression of hydrogen[4].

Ashcroft's hypothesis has been elaborated several times since. In 1989, for example, Marvin Cohen and his co-workers at the University of California at Berkeley carried out quantum-mechanical calculations of the strength of electron–phonon coupling in a high-pressure phase of hydrogen, from which they deduced that the superconducting T_c at around 400 GPa should be about 230 K (ref. 5). At that stage, such high pressures weren't accessible experimentally.

Ashcroft himself returned to the problem in 1997 (in fact, it seems never to have been too far from his mind), when he and C. F. Richardson showed that the superconducting behaviour depends crucially on whether the high-pressure phase is monatomic or retains the diatomic character of molecular hydrogen[6]. In the latter case, there are strong correlations between the electrons and holes in the electron bands that arise from overlapping orbitals, which enhance the electron pairing on which superconductivity depends. That boosts T_c even more, perhaps even to values of 400 K or so.

So what's new now? Pierluigi Cudazzo, at the Università deglie Studi dell'Aquila in L'Aquila, Italy, and co-workers, have looked again at the electron–phonon coupling in metallic hydrogen using *ab initio* quantum methods to figure out which are the main factors driving superconductivity[1]. They confirm that the electron–phonon interaction is strong, and say that the complex Fermi surface — the 'shape' of electron bands in momentum space — offers plentiful opportunities for electrons to couple. Most strikingly, their predicted T_c of 242 K at 450 GPa matches closely the cruder, earlier predictions, affording some confidence that, if only the experiments can be arranged, we'll find that superconductivity near room temperature is truly possible.

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