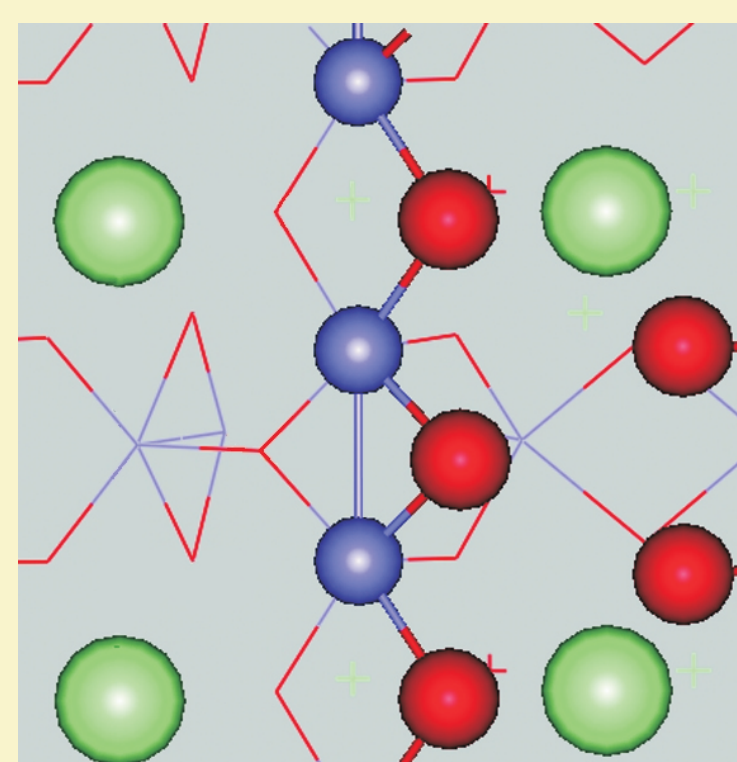


## Platí barat

In the continuing search for cheaper, more efficient catalysts for cleansing diesel engine exhaust, researchers report a new class of mixed-phase oxides that under laboratory conditions exceed the performance of expensive commercial platinum-based catalysts (*Science*, **2012**, 337, 832). A team of scientists report that Mn-mullite(Sm, Gd)Mn<sub>2</sub>O<sub>5</sub>—manganese-mullite materials containing either samarium or gadolinium—converts the toxic diesel engine exhaust product nitric oxide to the more benign nitrous oxide. The researchers investigated the catalyst's mechanism using infrared Fourier transform spectroscopy as well as density functional theory calculations. They found that its catalytic activity is localized at Mn–Mn dimers on the rough, defect-riddled, or “stepped” mullite surface. The catalyst might find use in so-called lean-burn engines, which use much less fuel than traditional internal combustion engines. Emissions control systems in these engines are costly and limit their commercialization. The new work may provide a solution for cost-effective lean gasoline emission control.



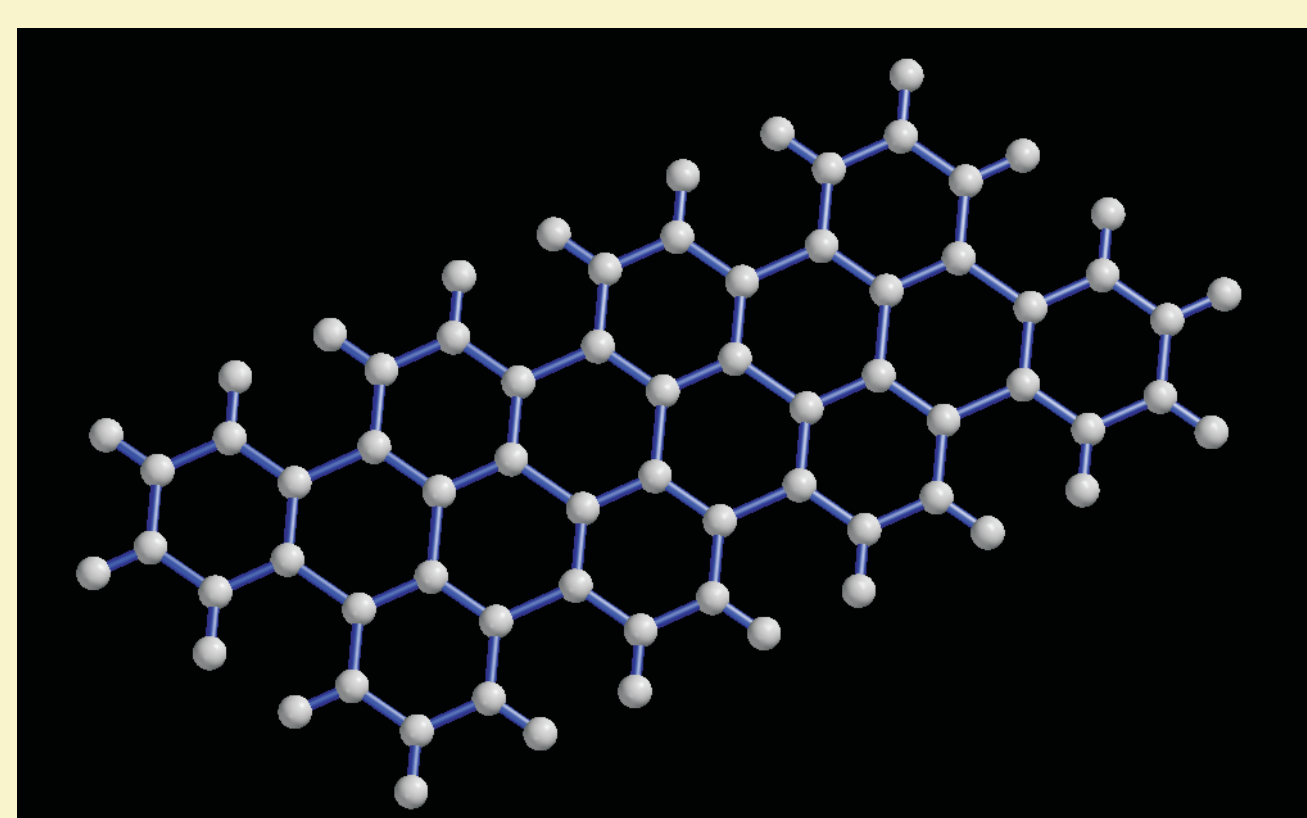
Simulation shows top view of the defect-riddled crystal surface of a new metal-oxide catalyst (O = red, Mn

## L'hidrogen imita el grafè

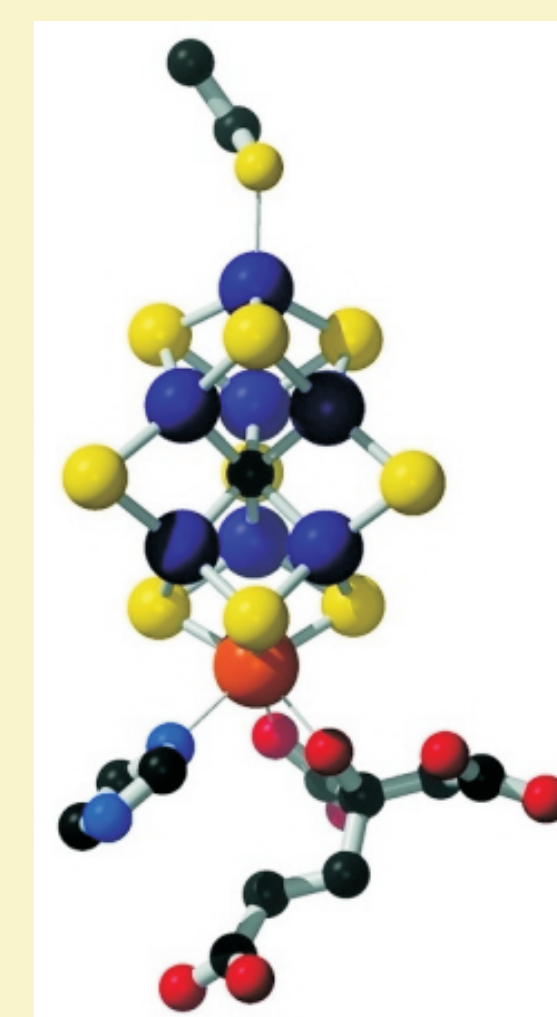
Researchers in the UK and the US claim to have discovered a new phase of hydrogen in which the diatomic molecules break apart to form six-atom rings, similar to graphene. The new phase, which occurs at very high pressures, could be a stepping stone towards a long-sought after phase: metallic hydrogen. The quest for metallic hydrogen has been on since the late 19th century, when chemists pointed out that the element, which tops the periodic table's column of alkali metals, ought to form a metal.

The challenge of metallic hydrogen is alluring because it has the potential for significant applications. For example, some believe this material could lead to a room temperature superconductor. The researchers subjected samples of hydrogen and deuterium to pressures up to 315 GPa in a diamond anvil cell at temperatures of 300 K. Using Raman spectroscopy, they measured the vibron frequency, which determines the strength of the H-H bonds and which therefore describes how 'molecular' the hydrogen is.

At 220 GPa, the researchers found that the main vibron frequency rapidly decreased, while a second vibron appeared, maintaining the original frequency. To understand these results, Gregoryanz's group turned to a theory of solid-hydrogen phases published in 2007 by physicists Chris Pickard and Richard Needs in the UK. One of the physicists' predictions for a new phase closely matched the latest results: graphene-like layers of hydrogen in irregular six-atom rings, which would explain the low vibron frequency, interspersed with unbound hydrogen molecules, which would explain the second, higher vibron frequency. At higher pressures, Gregoryanz says, these graphene-like layers may become symmetrical, and exhibit semi-metallic behaviour. (R T Howie et al. *Phys. Rev. Lett.*, **2012**,



## Un carbur al cor de la nitrogenasa



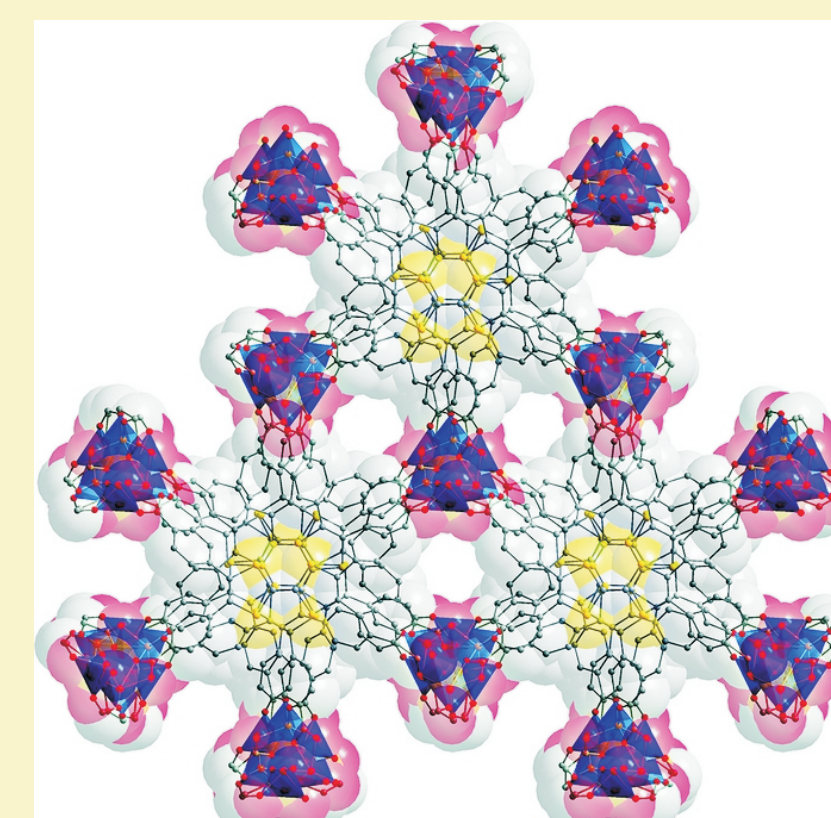
In the nitrogenase FeMo cofactor, a carbide ion (black sphere, center) coordinates to six of the seven Fe ions (purple). Mo is the large orange sphere, homocitrate is at bottom right, and protein ligands are at top and bottom left.

In an effort to better understand nitrogenase—the essential biocatalyst that bacteria use to convert N<sub>2</sub> into ammonia—researchers have now solved a mystery concerning the origins of a carbide ion in the enzyme complex. The work could lead to engineered versions of the enzyme that catalyze nitrogen fixation and related reactions for industrial applications such as ammonia production. A decade ago, it was discovered that a light atom of unknown identity in nitrogenase's FeMo cofactor, the enzyme's catalytic center. The atom seemed important because it was bonded to six of the cofactor's seven iron atoms. Last year, two groups showed independently that the mystery atom is carbide (C<sup>4-</sup>). Such carbide-iron species are extremely rare in biological metal centers.

Now, a group of researchers have nailed down the origins of the carbide. To do so, they linked NifB to another complex, NifEN. This linkage stabilized NifB, enabling them to show that NifB transfers carbide from S-adenosylmethionine to the FeMo cofactor during biosynthesis and to describe possible carbide-insertion mechanisms (J. A. Wiig, et al. *Science*, **2012**, 337, 1672). This fundamentally advances our understanding of a very complex process, as the FeMo cofactor is the most complicated biological metal cluster we know. Further research in this area could put to rest remaining questions about how the FeMo cofactor is assembled. It could also provide answers to the big questions of how and where on the FeMo cofactor the nitrogenase reaction actually takes place.

## MOF conductors

A new sulfur-and-zinc-based metal-organic framework (MOF) compound conducts charge nearly as well as the most conductive organic semiconductors, a team of researcher (M. Dinca et al. *J. Am. Chem. Soc.*, **2012**, 134, 12932). The study demonstrates that a typically nonconducting family of materials can be tuned synthetically to conduct charge, an advance that may lead to applications in electrochemistry and electronic materials. MOFs are crystalline materials composed of metal ions or clusters that are connected by organic linker groups. The materials' extreme surface areas and porosities have led to numerous record-breaking demonstrations and some commercialization of MOFs in gas separation and storage applications. Strategies to boost the conductivity of MOFs, for example by using linkers that mediate covalent interactions with metal ions, have been largely unsuccessful. To resolve those problems, the researchers drew upon studies showing that tetrathiafulvalene (TTF), an organosulfur compound, can form -stacked columnar structures, a feature that makes some materials good electronic conductors. The aim of the team was to use TTF groups to prepare a stable porous compound in which -stacked columns could provide a conduit for charge mobility. The strategy paid off. The group coupled TTF with a bromobenzoate compound; a measure of conductivity, in the material is comparable to that of common organic semiconductors.



**HOLEY CRYSTALS**  
 This depiction of the framework compound highlights its benzoate-lined pores (blue = Zn-based units, yellow = S, red = O, gray = C).

**Breus** • Científics japonesos diuen haver preparat l'element 113 (Ununtri, Uut), a partir de Zn i Bi (*J. Phys. Soc. Jpn.*, **2012**, 81, 103201). Els resultats estan pendents de confirmació per part de la IUPAC; és la quarta vegada que es dona informació sobre la síntesi d'aquest element.

• La IUPAC ha aprovat l'existència de l'enllaç d'halogen i el defineix com la interacció no covalent entre una zona positiva d'un halogen i una de negativa d'un parell solitari del nitrogen o l'oxigen. S'espera que serà especialment útil en camps com els materials i la biologia. (*Chem. Eng. News.*, **2012**, 90(35), 36)

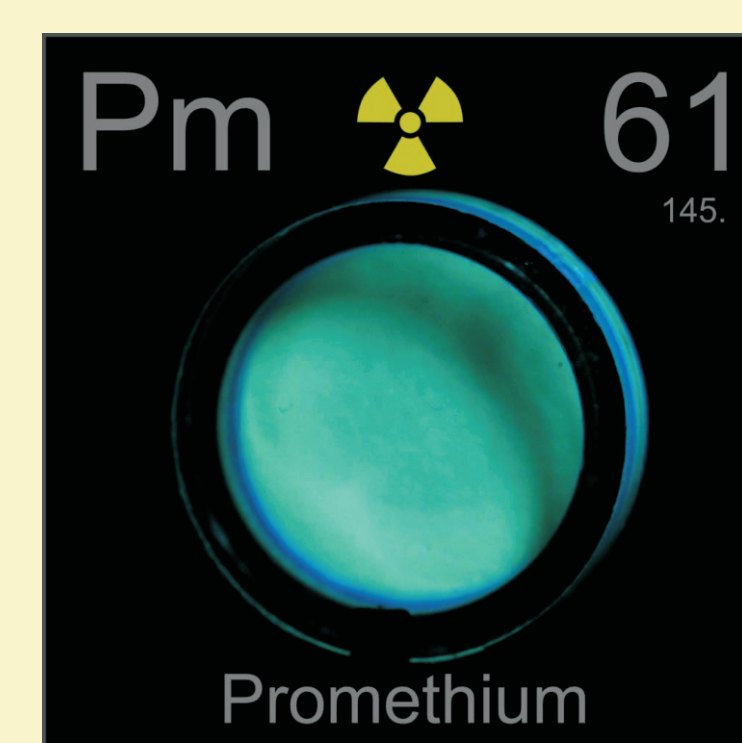
• Un equip de científics de diferent institucions, entre elles la UB, han demostrat que pintures rupestres del nord de la Península Ibèrica tenen un antiguitat de més de 40000 anys, fet que planteja la possibilitat que en la seva creació hi haguessin participat neandertals (*Science*, **2012**, 336, 1409)

## Avui recomanem

«*Voices of Inorganic Chemistry*», una sèrie de 12 vídeos que la revista *Inorganic Chemistry* ha editat amb motiu del seu 50è aniversari. Consten d'entrevistes, de quasi una hora de durada, amb químics de prestigi i reconeixement internacional.

<http://pubs.acs.org/page/inocaj/multimedia/voices.html>

## L'element

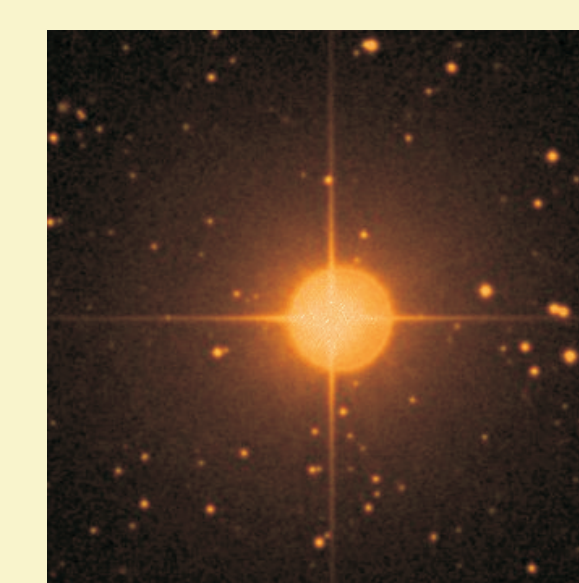


L'element número 59, el **prometi**, és un dels escassos elements lleugers de la Taula que té tots els isòtops radioactius i només es troba com a traces a la naturalesa. El seu nom prové del delu grec *Προμηθεύς*, que vol dir previsió i que entre altres mites és conegut per haver retornat el foc als homes.

Després de diferents propostes, la seva existència no fou confirmada fins el 1947 per J. A. Marinsky, L. E. Glendin i C. D. Coryell, als EUA, en tractar residus de fissió de l'urani.

Pertany al grup dels lantànids i té les propietats químiques característiques d'aquest grup d'elements. El Pm-147 és l'únic isòtop comercial, s'empra en pintures lluminoses com la mostrada a l'esquerra, composta per ZnS i traces de PmCl<sub>3</sub>; també en bateries atòmiques i en aparells per determinar gruixos. Aquest isòtop s'obté bombardejant U-235 amb neutrons tèrmics.

Com a curiositat val a dir que no s'ha detectat en els sistema solar, però sí a l'espectre de l'estrella HR465, a la constel·lació d'Andròmeda.



Imatge de l'estrella HR465 (GY Andromedae)