UNIVERSITAT DE BARCELONA
Química Inorgànica

Notícies Inorgàniques

Any 7, Núm. 39, Maig de 2008

http://www.ub.es/inorgani/dqi.htm

Editors: Gabriel Aullón, Ramón Bosque i Joaquim Sales. Correspondència: noticies@qi.ub.es

Les perovskites alteren la rotació terrestre

The possible existence of a highly conducting mineral layer just above the boundary between Earth's core and mantle has gotten earth scientists a little excited. Such a layer would, by electromagnetic coupling, have a small influence on the exchange of angular momentum between the planet's rotating fluid core and its solid mantle.

Theorists say this tiny difference could explain why the length of an Earth day fluctuates by a millisecond or so year-to-year and could contribute ever so slightly to Earth's wobbling axis of rotation. Kei Hirose and Kenji Ohta at Tokyo Institute of Technology and coworkers present a chemical model that provides the first direct conductivity measurements of the proposed mineral *(Science* **2008,** *320*, 89).

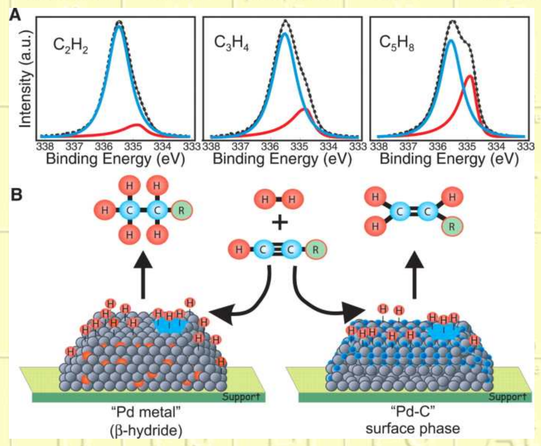
The team prepared samples of perovskite and tested its electrical conductivity. At the high temperature and pressure expected at the core-mantle boundary, the mineral underwent a phase transition. This transition is accompanied by a shift in the electronic structure of metal atoms, causing the conductivity to jump by two orders of magnitude.

En catàlisi, la *subsuperfície* és important

Catalysis is generally thought of as a surface phenomenon, yet a new study demonstrates that what happens several atomic layers below the catalyst surface can have a big impact on catalytic reactions.

Detre Teschner at the Fritz Haber Institute (Berlin), and colleagues show that the atoms just beneath the surface of a palladium catalyst help determine if alkyne hydrogenation proceeds selectively to an alkene or proceeds nonselectively all the way to an alkane *(Science* **2008,** *320*, 86).

The group has monitored the carbon and hydrogen content in palladium during catalysis. They found that when palladium indiscriminately hydrogenates alkynes to alkanes, far fewer carbon atoms are dissolved in the catalyst's subsurface. This result suggests that not only the surface but also the subsurface region is affected by the chemical potential of the reaction mixture.

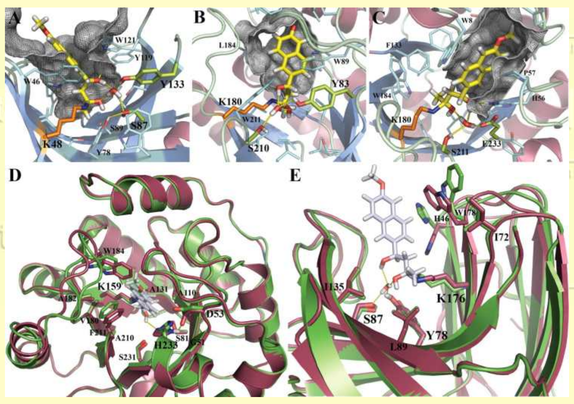


Enzims dissenyats per ordinador

In a dramatic example of translation from *in silico* to *in vitro*, scientists have computationally designed a series of new enzymes that catalyze a multistep reaction-including the breaking of a carbon-carbon bond-in laboratory experiments.

The designed enzymes, which catalyze the reverse of an aldol condensation reaction, aren't nearly as active as naturally occurring enzymes that perform similar tasks (D. Baker and coworkers, *Science* **2008**, *319*, 1387).

The researchers used the Rosetta protein structure prediction program to design a library of enzymes with active sites likely to catalyze the retro-aldol reaction. They whittled down a virtual list of more than 180,000 candidates to a promising 72. The team then synthesized those enzyme candidates in the lab. Thirty-two enzymes catalyzed the reaction; some accelerated the reaction rate by up to four orders of magnitude.

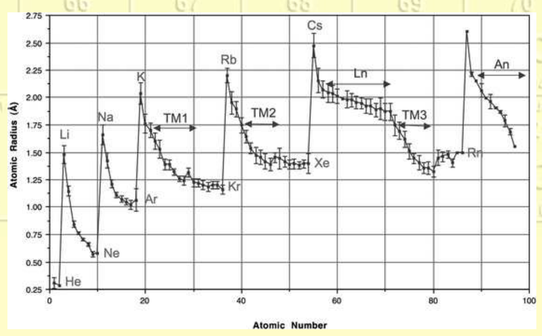


Radis *made in* UB

A new set of covalent atomic radii that is more comprehensive and precise than previous lists has been compiled by scientists from the Universitat de Barcelona (S. Alvarez and coworkers, *Dalton Trans.*, **2008,** 2832).

The concept of atomic radii is used in structural chemistry and crystallography to give a rough idea of the size of an atom in a molecule or crystal, and to establish bonding and non-bonding interactions between atoms. The new list of radii covers elements up to curium (atomic number 96) and shows sensible trends along both the rows and groups of the periodic table.

The Spanish team derived their radii from a systematic search of 228 000 experimental bond distances in structures held in the Cambridge Structural Database (CSD) and the Inorganic Crystal Structure Database (ICSD). They determined the radii from bond distances to nitrogen, carbon and oxygen atoms, as there many examples of covalent bonds from these to most other elements.



Breus

• A Almeria s'ha instal·lat el parc d'energia solar més gran del món per produir hidrogen a partir de l'aigua. S'espera que el procés sigui competitiu en uns 10 anys.

http://www.psa.es

• La policia de Singapur està fent servir l'espectroscopia Raman per dur a terme estudis forenses. L'anàlisi de fragments d'ungles permet determinar el sexe de la persona, i detectar també diferents malalties (E. Widjaja *et al.*, *Analyst*, **2008,** 133, 493).

• Una confusió entre $MgSO_4$ i $MnSO_4$ en l'etiquetatge d'un medicament sembla que ha estat responsable d'un accident fatal a Catalunya.

Avui recomanem

El proper 18 de juny a les 11 hores, a l'aula magna Enric Casassas de la Facultat de Química, tindrà lloc un homenatge al Dr. Joan M. Coronas (1912 - 2007), primer Director del Departament de Química Inorgànica.

L'element

L'element número **39**, **itri,** fou descobert per Johan Gadolin l'any 1794 en el mineral gadolinita, a Ytterby (Suècia). Fou aïllat per F. Wöhler l'any 1828 per reducció del YCl_3 amb potassi. És el primer element de les terres rares, i els seus òxids –en especial Y_2O_3 i derivats– tenen aplicacions tecnològiques importants com la fabricació de granats útils com a gemes, en la transmissió de so, làsers, filtres de microones, LEDs i de materials superconductors.