

La intimitat d'un catalitzador

Researchers of catalan universities (J. Llorca (UPC), N. Divins (UPC), I. Angurell (UB), C. Escudero (ALBA), and V. Perez-Dieste (ALBA), *Science*, **2014**, *346*, 620; DOI: 10.1126/science.1258106) have discovered the way the atoms move in a real catalyst and have shown that they react in different ways according the support.

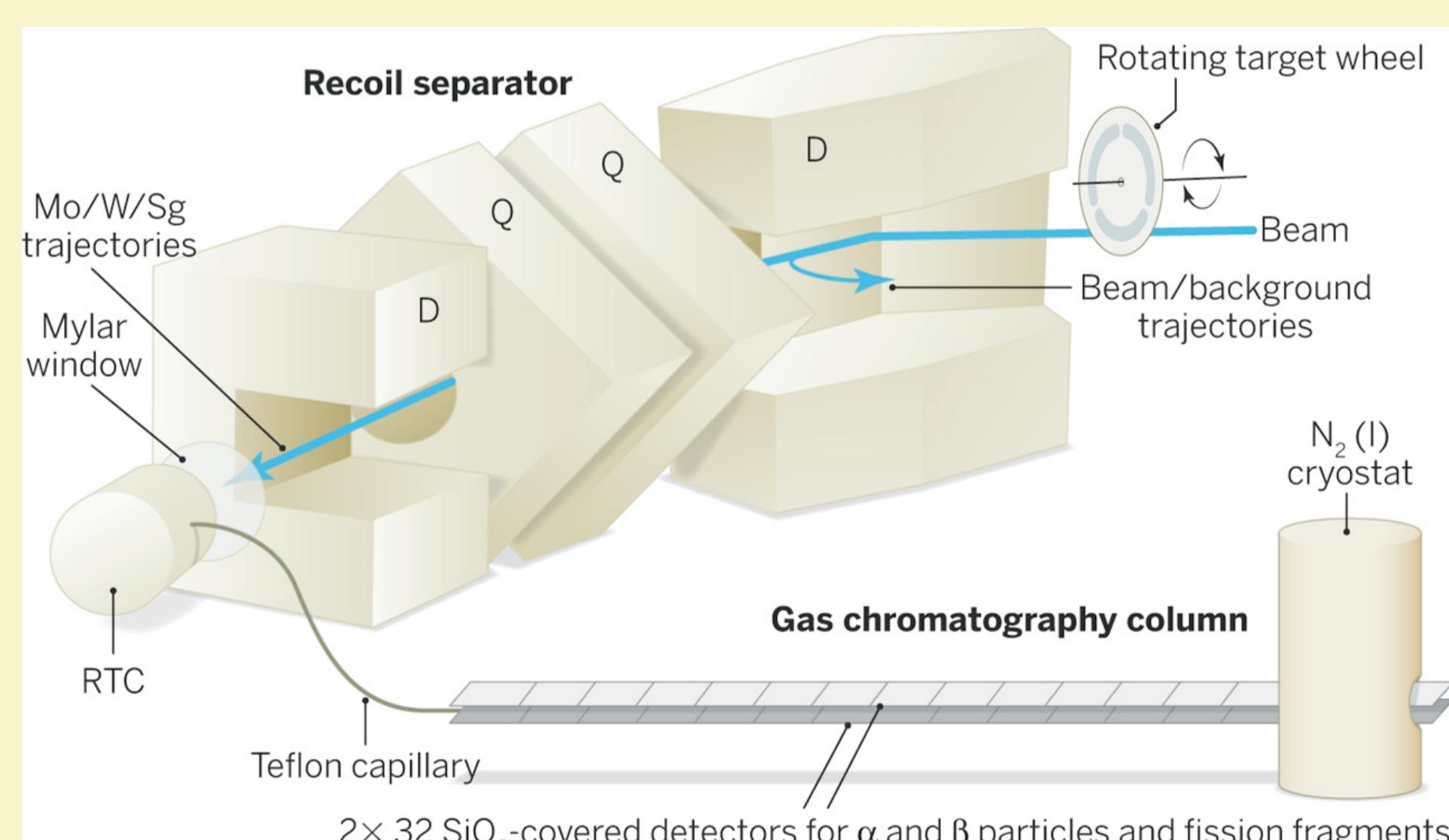
Catalysts used for heterogeneous processes are usually composed of metal nanoparticles dispersed over a high-surface-area support. In recent years, near-ambient pressure techniques have allowed catalyst characterization under operating conditions, overcoming the pressure gap effect. However, the use of model systems may not truly represent the changes that occur in real catalysts (the so-called material gap effect). Supports can play an important role in the catalytic process by providing new active sites and may strongly affect both the physical and chemical properties of metal nanoparticles. The authors of this work used near-ambient pressure x-ray photoelectron spectroscopy to show that the surface rearrangement of bimetallic (rhodium-palladium) nanoparticles under working conditions for ethanol steam reforming with real catalysts is strongly influenced by the presence of a reducible ceria support.



Rhodium-palladium nanoparticles supported on CeO_2

El seaborgi es comporta com cal

Scientists have succeeded in creating 18 molecules of a seaborgium carbonyl complex, $\text{Sg}(\text{CO})_6$. Seaborgium and other transactinides can be created only in particle accelerators, but studies of their chemistry help determine the accuracy of chemical theory and whether an element's position in the periodic table correctly reflects its reactivity. The properties of transactinides are uncertain because those elements are subject to relativistic effects in which the innermost s orbitals contract, outer d and f orbitals expand, and electron energy levels split as a result of spin-orbit coupling—all affecting an element's reactivity. A team working at Japan's RIKEN Nishina Center for Accelerator-Based Science (Ch. E. Dülman et al., *Science* **2014**, *345*, 1491; DOI: 10.1126/science.1255720) created $\text{Sg}(\text{CO})_6$ by bombarding a ^{248}Cm target with ^{22}Ne and then magnetically separating seaborgium and its group 6 neighbors molybdenum and tungsten from other products. They next treated the metals with carbon monoxide and funneled them to a silica gas chromatography column lined with radiation detectors to identify the species. $\text{Sg}(\text{CO})_6$ adsorption to the column was similar to $\text{Mo}(\text{CO})_6$ and $\text{W}(\text{CO})_6$ adsorption, which the researchers say confirms theoretical predictions.



Breus • Els Premis Nobel de Química d'enguany han estat atorgats a Eric Betzig (Howard Hughes Medical Institute, Ashburn, Virginia), Stefan W. Hell (Max Planck Institute for Biophysical Chemistry, Göttingen) i William E. Moerner (Stanford University, California) pel desenvolupament de la microscòpia de fluorescència d'alta resolució. El de Física ha estat per a Isamu Akasaki (Nagoya University), Hiroshi Amano (Nagoya University) i Shuji Nakamura (University of California, Santa Barbara), per la invenció de LEDs molt eficients. (www.nobelprize.org). El lliurament tindrà lloc a Estocolm, el proper 10 de desembre.

- S'ha preparat un compost amb tots els elements, excepte el Ne, del bloc 2p: FBNCO. De moment només s'ha aïllat a l'estat gasós i no és gaire estable, es descompon als 0.8 μs . (A. Troiani et al., *Chem. Commun.*, **2014**, *50*, 13900; DOI: 10.1039/c4cc05217j).

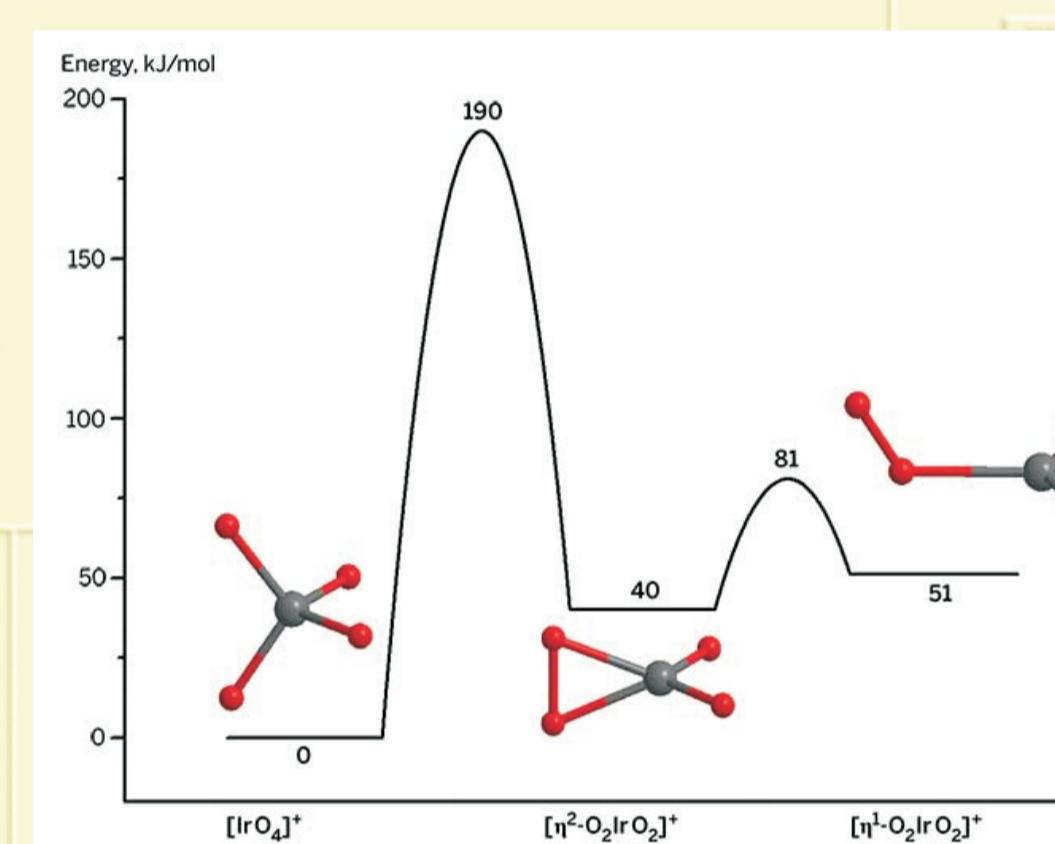
- L'empresa Merck ha comprat Sigma-Aldrich per 13.000 milions d'euros; el catàleg resultant tindrà més de 300.000 productes.

Avui recomanem

La Mostra del Fons Històric de la Biblioteca de Física i Química, que arriba a la desena edició, està dedicada enguany a «Cristalls a la llum dels Raigs X», coincidint amb el centenari de la concessió del Premi Nobel a Max von Laue l'any 1914 i als Bragg, pare i fill, l'any 1915.

L'iridi arriba al 9!

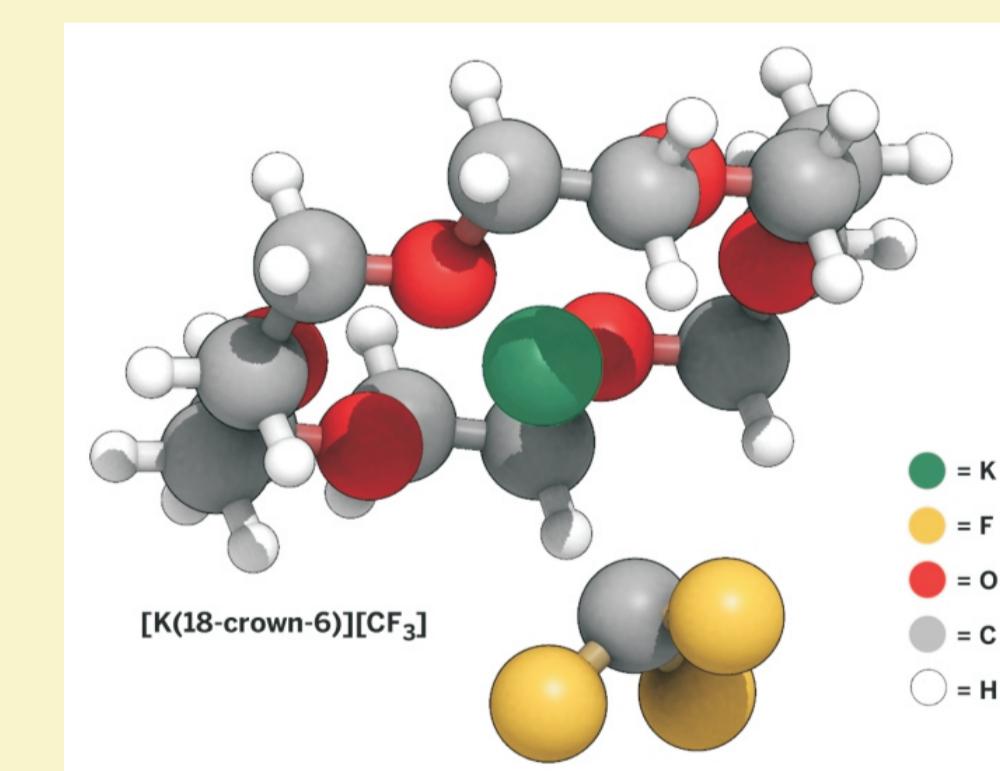
The oxidation state of an atom in a molecule is an important means of electron bookkeeping and determining structure and bonding, so the question of just how high oxidation states can go has long piqued chemists' interest. That ceiling has now reached what was once believed to be an impossibly high level with the preparation of IrO_4^+ , the first example of a molecule with an oxidation state of +9. The highest observed oxidation state had been +8, which occurs in only a few tetroxide compounds— RuO_4 , OsO_4 , IrO_4 , and XeO_4 . These are molecules in which the central atom has plenty of valence electrons to give away and the high charge can be stabilized by small, highly electronegative ligands such as fluorine or oxygen. Among the +8 molecules, IrO_4 stands out because the central iridium atom still has one more 5d valence electron to give. A team of researchers, have now coaxed iridium to go all the way (S. Riedel et al., *Nature* **2014**, *514*, 475; DOI: 10.1038/nature13795). To make IrO_4^+ , the group blasted an iridium metal target with a pulsed laser in an argon atmosphere spiked with O_2 . The researchers studied the reaction products by mass spectrometry and infrared photodissociation spectroscopy. By coupling experimental and computational modeling, the researchers determined that the most stable IrO_4^+ isomer has tetrahedral geometry and four terminal $\text{Ir}=\text{O}$ bonds.



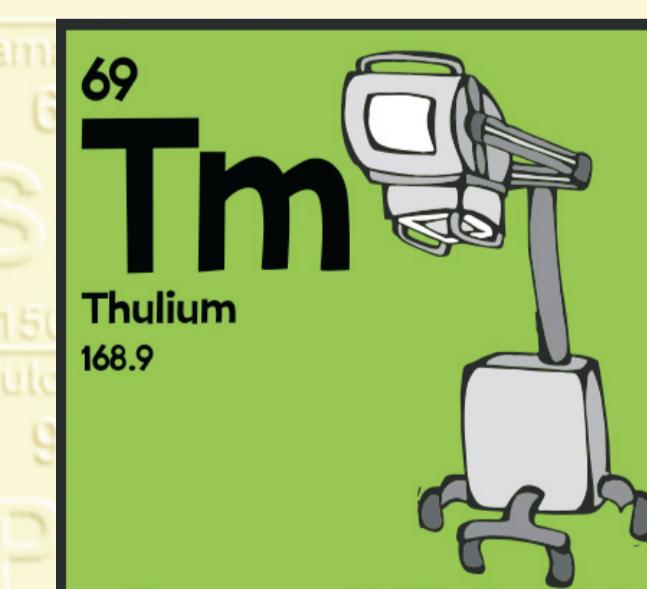
Calculated optimized structures and energetic ordering of three detected IrO_4 isomers; IrO_4^+ with iridium in the +9 oxidation state (left) is the most energetically favored isomer.

El trifluorometanur capture

For chemists, adding fluoroalkyl groups to molecules is an important way of controlling properties such as the bioactivity of drugs and the performance of plastics and electronic materials. The trifluoromethanide anion, CF_3^- , has long been the proposed key intermediate in these reactions, but no one has been able to trap the anion—it's been thought to only pop in and out of existence. Researchers at the University of Southern California now report capturing and studying a stable trifluoromethanide complex for the first time. The finding brings added clarity to trifluoromethylation reactions and is expected to help guide research and commercial efforts. Chemists have suspected that CF_3^- undergoes fast, reversible defluorination to form difluorocarbene and fluoride as part of its reactivity. But the researchers (G.K. Surya Prakash et al., *Angew. Chem. Int. Ed.* **2014**, *53*, 11575; DOI: 10.1002/anie.201406505) discovered through thermodynamics calculations that the anion should be persistent at low temperature. They then determined that the optimal way to stabilize trifluoromethanide would be to pair it with the right metal cation. Potassium topped the list, and the team proceeded to capture the anion in bulk amounts as a potassium crown ether complex and confirmed its existence through low-temperature NMR spectroscopy. The anion remains stable in solution for several days at -78°C .



L'element



L'element número 69, tuli, el descobrí el químic suec Per Theodore Cleve de la Universitat d'Uppsala l'any 1879, en un procés de purificació del Er_2O_3 , després d'haver-ne separat l'holmi (vegeu *Not. Inorg.*, **67**, Maig, 2104). El nom prové de "Thule", antiga denominació de Suècia. És el lantànid menys abundant, llevat del prometí que és un element artificial. Pur no fou preparat fins el 1911 pel professor de la Universitat de Harvard William Richards – guardonat amb el Premi Nobel de l'any 1914 per les seves contribucions a la determinació de pesos atòmics –, per cristal·lització fraccionada del seu bromat i després de més de 15.000 purificacions. La producció anual, com a òxid, és d'unes 50 Tm.

A pesar de la baixa abundància es coneixen algunes aplicacions, com en els granats Ho:Cr:Tm i Ho:Cr:Tm components de làsers emprats en meteorologia, en superconductors, i en aparells de Raigs X portàtils. La seva propietat fluorescent a la llum ultraviolada el fa útil com a components d'aparells per detectar bitllets falsos. Es troba present en quantitats molt petites en el cos humà i no se li coneix cap activitat biològica.