

## **The Route to Better Catalysts: From Surface Science to Nanotechnology**

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One of the major challenges in heterogeneous catalysis is the preparation of highly selective and robust catalysts. The goal is to be able to synthesize solids with stable surfaces containing a large number of specific surface sites designed for the promotion of a particular reaction. New synergies between surface-science studies and novel nanosynthesis methodology promise to afford new ways to design such highly selective catalysts in a controlled way. Here we will provide a progress report on several projects ongoing in our laboratory based on this approach. First, we will offer a general discussion on the unresolved issues associated with olefin-conversion reactions promoted by metal surfaces. In a specific project, platinum-based catalysts were designed for the selective trans-to-cis conversion of olefins based on early surface-science work with model single-crystal surfaces and quantum mechanical calculations that indicated a particular preference for (111) facets in promoting the formation of the cis isomers. A metal-nanoparticle encapsulation procedure was also developed to increase catalyst stability and to prevent sintering. In a second example, new metal@TiO<sub>2</sub> yolk-shell nanomaterials were conceived for both regular and photo-induced catalytic applications. These catalysts can promote CO oxidation at cryogenic temperatures, and suggest that in photocatalysis the role of the metal may not be to scavenge the excited electrons produced in the semiconductor upon absorption of light, as commonly believed, but rather to promote the recombination of the adsorbed atomic hydrogen initially produced by reduction of H<sup>+</sup> on the surface of that semiconductor. Additional examples will be briefly introduced, including the use of "click" chemistry to tether molecular functionality on porous solid materials, the use of self-assembly, sol-gel chemistry, and atomic-layer deposition (ALD) to prepare catalysts with well-defined structural characteristics, and the use of "single site" bimetallic catalysts to promote selective hydrogenations.

### **Biosketch**

Francisco Zaera received his Licenciata and PhD degrees from the Simón Bolívar University in Caracas, Venezuela (1979), and the University of California, Berkeley (1984), respectively. He was an Assistant Chemist at the National Synchrotron Light Source of Brookhaven National Laboratory from 1984 until 1986 before joining the University of California, Riverside, where he is presently a Distinguished Professor of Chemistry. He is also Senior Editor of The Journal of Physical Chemistry Letters. Zaera has authored over 400 articles in scientific publications, and has received several national awards, including the American Chemical Society George A. Olah and Arthur W. Adamson Awards, the North American Catalysis Society Paul H. Emmett Award, a Humboldt Research Award for Senior Scientists, and, this year, the inaugural ACS-CATL Exceptional Achievements in Catalysis. He is a Fellow of the American Chemical Society, the American Vacuum Society, and the American Association for the Advancement of Science. His research interests are in surface and materials chemistry and in heterogeneous catalysis. More information about Prof. Zaera can be found at <http://chem.ucr.edu/Zaera/lab.html>.