Model Catalysts from Single Crystals to Nanocrystals/Nano-Composites

CAS/MPG Partner Group on Structure-Activity Relation of Model Systems for Heterogeneous Catalysis
Hefei-Berlin, 2007.1.1 – 2011.12.31

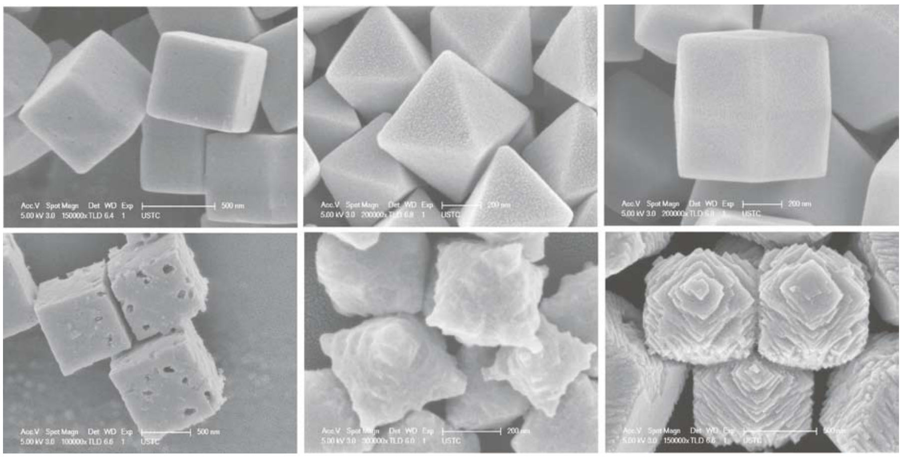
Leaders of the partner group, Prof. Hans-Joachim Freund (left) and Prof. HUANG Weixin (middle), with members of the mid-term evaluation committee Prof. Hans-Peter Steinrück (chairman, second left), Prof. YANG Jinlong (second right) and Prof. BAO Xinhe (first right).

Officially set up in 2007 by scientists from the University of Science and Technology of China (USTC), CAS in Hefei and the Fritz Haber Institute, MPS in Berlin, the Partner Group focused on the fundamental study of the structure-activity relation of solid catalysts via the model catalyst approach.

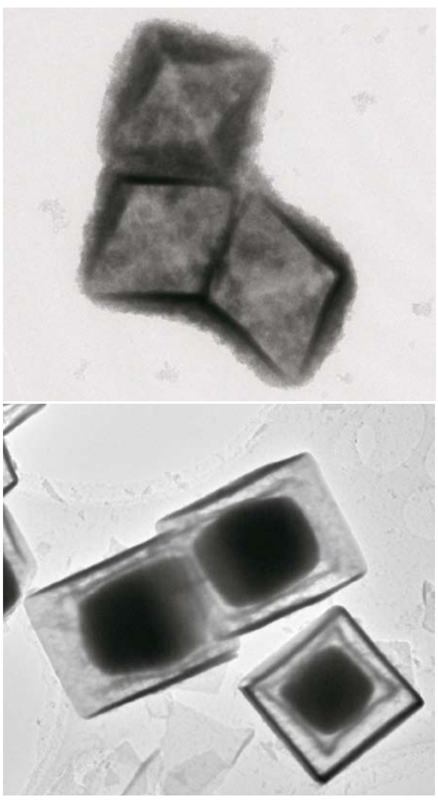
Reported by Group Leader HUANG Weixin

Heterogeneous catalysis is a key technology for chemical and materials synthesis, fuel production, power generation and conversion, and environmental remediation. To cope with resources (energy) shortage and environmental pollution, chemical processes should be not only efficient but also clean, and catalysts must be active and selective. The innovation of such catalysts requires a fundamental understanding of the structure-activity relation of catalysts that can guide the design of catalyst structures.

Photos/Images: By courtesy of Prof. HUANG Weixin.



As-synthesized Cu_2O cubes, octahedra, and rhombic dodecahedra (left to right, top images) expose different crystal planes and surface compositions, thus they exhibit different surface reactivity and morphological evolutions during oxidative dissolution reaction in HAc solution (bottom images).



The team successfully fabricated Cubic Cu_2O/CeO_2 core/shell nanocomposite (left) and void CeO_2 octahedra (right) via template-assisted method, employing cubic and octahedra Cu_2O polyhedra templates respectively under the same reaction conditions. The results demonstrate that morphology-dependent surface reactivities of cubic and octahedra Cu_2O polyhedra can be related to morphology-dependent exposed crystal planes and surface structures.

Heterogeneous catalysis always occurs on the surface of solid catalysts, so the surface composition, electronic structure and geometric structure of a solid particle jointly determine its catalytic property. Solid catalysts prepared by routine methods usually exhibit an inhomogeneity of catalyst particles in their sizes and morphologies, which makes the unambiguous correlation between the measured catalyst surface structure and catalytic property difficult. In this regard, the model catalyst approach, in which solids with uniform and well-defined surface are employed as model catalysts to establish the structure-catalytic property relation, has been proved as a successful approach. Besides, traditional model catalysts are mainly based on single crystals, single crystal thin films, and nanoparticles supported on single crystals/single crystal thin films. Benefiting from the recent significant progress of nanotechnology, nanocrystals and nanocomposites with uniform compositions and structures (including size and morphology) can be successfully prepared.

In our study, we use well-defined nanocrystals and nanocomposites as a novel type of model catalysts. The study of structure-activity relation employing nanocrystals/nanocomposites -based model catalysts can be carried out under the same experimental condition as practical heterogeneous catalytic reactions and thus can approach industrially-important fundamental questions in heterogeneous catalysis. Employing model catalysts from single crystals to nanocrystals/nanocomposites, we have studied the structure-activity of oxide catalysts and supported Au catalysts, and acquired a fundamental understanding of the oxygen vacancy-controlled reactivity of hydroxyls on oxide surfaces, the crystal plane-controlled surface reactivity and catalytic property of cuprous oxide catalysts, the structure-intrinsic activity relation of supported Au nanoparticles, and photocatalytic reaction mechanisms. More detailed information can be found at http://staff.ustc.edu.cn/~huangwx.

"What I have experienced is the generosity of my German partners in encouraging and supporting me in my early scientific career, and I have benefited from the cooperation very much."

— Prof. HUANG Weixin

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