UV Raman Spectroscopic Studies on Catalytic Materials

Due to their excellent work on UV Raman spectroscopic studies on catalytic materials, a team of scientists led by CAS Member Prof. LI Can at the Dalian Institute of Chemical Physics (DICP), CAS were awarded with a Second-Prize from the 2011 State natural Science Award. The team has long devoted themselves to the research on catalytic materials, and has helped solve some long-standing difficulties in this field, including the characterization of catalyst activity and studies into synthesis mechanisms of catalytic materials.

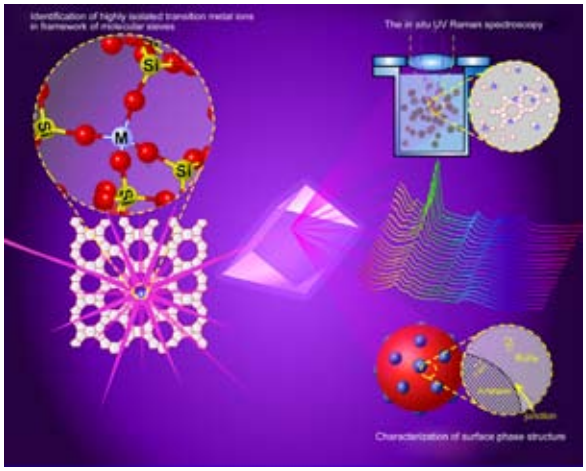
Characterization of catalyst activity, which plays a key role in studies of catalysis mechanisms, as well as the synthesis of catalytic materials have long baffled chemists. Highly active materials catalyze reactions at extremely low central concentrations; this makes it a terrifying mission to characterize the active sites and surface phase of them. The extreme conditions like high temperature and pressure involved in the synthesis of some catalytic materials like molecular sieves set a very high barrier for related research.

Innovations in new characterization techniques are thus called for to speed up breakthroughs in this field. Raman spectroscopy, amid the development of catalysis, nanotechnology and material science, has been employed as a powerful tool to studying the structure and identifying active sites of heterogeneous catalysts as well as solid materials. Conventional Raman spectroscopy, however, often failed due to strong fluorescence interference. Answering this challenge, LI's group at DICP successfully bypassed the interference in visible Raman and obtained enhanced Raman signal with their invention of UV Raman spectroscopy, smartly taking advantage of the shorter wavelength and the resonance Raman Effect at UV frequencies.

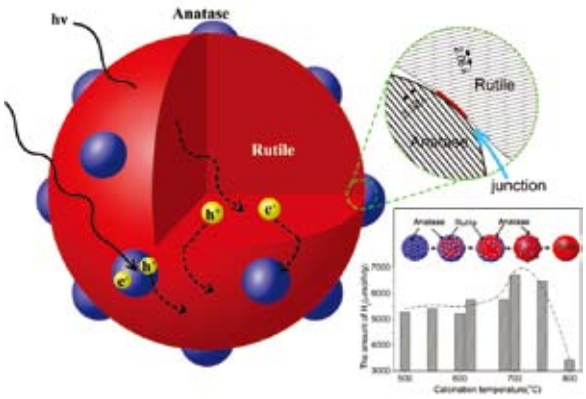
Based on their successful development of new methods for characterization of catalytic materials, the team revealed the crucial conversion processes and key intermediates with active sites, and proposed a theory for the formation mechanism of catalytic materials. Their work provides an experimental and theoretical basis for the rational design and preparation of novel catalytic materials at a molecular level.

UV Raman spectroscopic technologies for catalytic materials invented by CAS Member LI Can's team.

Building on their own UV Raman instrument and *in situ* UV Raman techniques, the team succeeded in characterizing various catalytic materials. For the first time, they identified highly isolated transition metal ions incorporated in the framework of zeolite at extremely low concentrations, based on the UV resonance Raman Effect. The UV Raman spectroscopy is also sensitive to surface phase transitions, which makes it particularly applicable for nano-scale particles that absorb UV light. Starting from this, the team established the relation between the photocatalytic activity of TiO_2 nanoparticles and their surface-phase structure. Using *in situ* UV Raman spectroscopy, they successfully elucidated the synthesis mechanism of zeolites



The team applied its own invention, the UV Raman spectroscopy to catalytic materials characterizations and produced a series of new results, including the identification of highly isolated transition metal ions incorporated in zeolites framework at extremely low concentration, and the elucidation of the synthesis mechanism of zeolites under real synthesis conditions via *in situ* UV Raman spectroscopy.



The team studied the surface anatase phase and rutile phase of TiO_2 semiconductor nanoparticles, and revealed the fact that the surface phase junction of semiconductor nanoparticles can enhance its photocatalytic activity.

under real synthesis conditions, solving issues including the identification of primary units, assembly through key intermediates, transition metal species, and the roles played by organic templates in framework formation.

The research has published about 100 peer-reviewed papers in international journals including *Angew. Chem. Int. Ed., J. Catal., Chem. Eur. J.*, and *J. Phys. Chem, etc.*, with 1972 citations, and five patents granted. Particularly, the work on the relationship between surface hetero-phase junction and the photocatalytic activity of semiconductors was published in *Angew. Chem. Int. Ed.* and *J. Am. Chem. Soc.*, highlighted by *Chemical & Engineering News* in its "Sci. & Tech. Concentrates" section (*Chemical & Engineering News*, 2008: 86, 25). Their finding has been considered as a strategy to develop high-activity photocatalysts for both environmental protection and solar energy utilization. The UV Raman spectroscopic study on transition metal substituted zeolite and zeolite synthesis mechanism was highlighted as one of the most important advances in the field of zeolite research by the 15th International Zeolite Conference held in Beijing, 2007, and the authors were invited to publish review papers in the *Journal of Catalysis* for its 40th anniversary, and in other distinguished peer-reviewed journals such as *Accounts of Chemical Research*, and *Chemical Society Review*.

One of the co-authors, CAS Member Prof. LI Can, the principal scientist of the project, was invited to give over 20 keynote/plenary lectures at international conferences including the plenary lecture at the 13th International Congress on Catalysis (ICC) in Paris, 2004, and awarded the prestigious International Catalysis Award at this conference. Due to his significant contributions to catalytic science and technology including the UV Raman spectroscopic study on catalysis, LI was highly recognized by both national and international scientific communities, and was selected as Member of CAS in 2003, Member of the Academy of Sciences for the Developing World (TWAS) in 2005, and Foreign Member of *Academia Europaea* in 2008. He is currently Director of the State Key Laboratory of Catalysis based in DICP, Chairman of the Catalysis Society of China and President of the International Association of Catalysis Societies. He was invited as an Associate Editor to the *ChemComm* Editorial Board, and an editorial member of over ten international journals. The team's invention, the UV Raman spectroscopic technique has been commercialized by a scientific instrument company in Beijing, China.

Main contributors to the project (from left to right): Profs. FENG Zhaochi, LI Can, and YANG Qihua.