

## Preface



The subject of international conference “Physical Methods for Catalytic Research at the Molecular Level”, devoted to the memory of academician K.I. Zamaraev and scheduled to its 60 years anniversary, reflected his research interests, such as catalysts investigation on atomic–molecular level and application of phys-

ical methods, especially spectral, for its purpose:

- quantum chemical studies of the electron structure of catalyst active components and molecular adsorption on active sites;

- physical methods used to investigate the surface and adsorption processes;
  - active sites on the surface of heterogeneous catalysts and elementary mechanisms of involved heterogeneous reactions;
  - elementary mechanisms of homogeneous catalytic reactions;
  - development of new methods to study catalysts in situ.
- investigation of active catalyst sites with the different kinds of spectroscopy using various probe molecules;
  - investigation of intermediates and meta-stable structural species, existing on the catalyst surface only under reaction conditions, with various in situ methods.

The conference was attended by 177 participants from 15 countries, and Russia was presented by the largest delegation.

In whole, presented were 12 plenary lectures, 12 special subject lectures, 32 oral reports and 98 posters.

Most presentations discussed the experimentally studied structure of catalyst-active sites, as well as the mechanisms of heterogeneous and homogeneous catalysis, investigated with physical methods.

The atomic molecular description of catalysts and related processes is one of the determining trends in the modern theory of chemical catalysis. It reveals the local character of reagents' interaction with the catalyst, and introduces a new concept of active sites (particular atomic-molecular species), working on the active catalyst surface. This opens wide possibilities for the use of physical methods to study the structure of active sites and intermediates, participating in some catalytic transformations. One may distinguish the following principle directions of physical methods application to research in catalysts:

- investigation of atomic-molecular structure of catalysts during their synthesis and treatment under thermal-vacuum or redox conditions; for the purpose that one commonly uses X-ray phase and HREM analysis, X-ray electron and photo-electron spectroscopy, IR, UV and NMR spectroscopy, including the Raman and Mössbauer methods, as well as neutron studies, which become rather popular;

Quantum chemical calculations appear to be a powerful tool of recent research attention owing to their improved prediction ability regarding the structure of active sites and catalysis mechanisms. Combined with spectral and kinetic methods, they open new perspectives for molecular theory in catalysis.

In whole, the conference was well represented in all abovementioned research fields. On importance is that Russian works, performed with physical methods, conform to the world standards regarding ideology and creativity. Modern equipment supply is the most critical factor for the Russian scientists due to the well-known economic crisis in Russia. However, at present, many leading Russian research teams work in a tight cooperation with foreign universities and institutions well supplied with the most advanced equipment.

Estimating the results, obtained with physical methods and presented at the conference, one may understand that in most cases, physical methods provided a better and qualitatively new understanding of catalysts' performance. Thus, NMR method helped the identification of such intermediates as singlet oxygen among the products of hydrogen peroxide decomposition in the presence of ions in configuration  $d_0$  such as Mo (IV), W (VI), V (V) (I.I. Voiseeu), acid catalysis intermediates in zeolites and intermediates produced in the course of alkanes dehydrogenation over Ga and Zn containing zeolites (E.G. Derouane), intermediates in the epoxidation of hydroperoxo- and alkylperoxo-complexes of transition elements, and intermediate structures in the synthesis of zirconocene polymerization catalysts (E.P. Talsi). Advanced MAS and NMR techniques expanded research abilities in study-

ing nuclei with a quadrupole moment, as was demonstrated with vanadium supported catalysts.

The capacity of IR spectroscopy was discussed in relation to adsorption–desorption processes and elucidation of reaction limiting stages (E.A. Paukshtis). DRIFT spectroscopy was found to be efficient in studying cation sites in zeolites, and in situ DRIFT was used to characterize the intermediates in methanol reforming over Cu–ZnO–ZrO<sub>2</sub>–Al<sub>2</sub>O<sub>3</sub> catalysts. Laser Raman spectroscopy attracts a growing recent attention of catalysis researchers, and promises most fruitful results if applied in situ.

X-ray and XPS methods continue to be widely used in catalytic research, but data interpreting still remains one of the most complicated actual problems.

Accumulated experience allows one to analyze the role of distortions and defects in the regular catalyst structure relevant for the EXAFS data interpreting (D.I. Kochubey). TEM and HREM studies meet wider and wider application in catalysis. Some reports were dedicated to STM application for studying catalysts surface, adsorption and surface processes (E. Eltsov, Sh. Shaikhutdinov), or for discussing the results obtained with this method in conjunction with the data of other methods (Ya. Iwasawa). X-ray structural studies traditionally occupy stable position in catalysis (E.M. Moroz, L.D. Marks). Most often real success was obtained with a combination of various physical methods. Thus, this approach helped to characterize the role of various phase structures in many component catalyst for olefins oxidation, to compare the contribution of primary and secondary reactions in the oxidative dehydrogenation of propane on supported vanadium oxide, to find the structure of newly synthesized oxide catalysts for the high-temperature oxidation (A.G. Anshits), to elucidate the influence of weakly adsorbing molecules (gas phase) on the catalytic reaction mechanism (Ya. Iwasawa), to characterize the structural sites of supported Pt/Al<sub>2</sub>O<sub>3</sub> catalysts, and so on. Let us mention a

newly developed method based on the high temperature differential scanning calorimetry in situ, and acoustic waves spectroscopy (S.Z. Yao).

Theoretical studies involved calculation methods specially developed for studying reaction kinetics on the catalyst surface (V.I. Elokhin), a well grounded new approach in a quasi-classic description of quantum dynamics related to low-temperature reactions, and some quantum chemical studies related to particular systems (E. Golubeva, A. Lamberov, I. Yudanov, M. Milov, N. Kachurovskaya).

Physical methods for research in situ encompass one of the most actual problems, which are met in the development of molecular theory in catalysis. This aspect was discussed by Prof. R. Shloegl, who attracted attention to meta-stable structures forming at catalytic transformations such as selective methanol oxidation on metal silver and copper catalysts. Spectral methods, combined with kinetic and quantum chemical studies, open other promising ways. Various methods, used to study some particular systems, traditionally give fruitful results, but may provide even more interesting data, if used together with molecular modeling.

Considering the fact that many Russian and foreign scientists are interested in the conference subject and that only Gordon conferences arranged in the USA regularly discuss the abovementioned problems in a concentrated form, the participants of International Zamaraev Conference “Physical Methods for Catalytic Research at the Molecular Level” recommended to arrange this conference once in 4 years in different countries.

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