Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
Zelinsky Institute of Organic Chemistry RAS, Moscow, Russia
Lomonosov Moscow State University, Moscow, Russia

MCR 2016

X International Conference "Mechanisms of Catalytic Reactions"

Svetlogorsk, Kaliningrad Region, Russia
October 2 - 6, 2016

ABSTRACTS

Novosibirsk-2016

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Topics of book:
- First-principles approach, theory and simulation in catalysis;
- Advanced methods for studies of mechanisms of catalyzed reactions;
- In-situ and operando studies of model and real catalysts;
- Kinetics and reaction intermediates of catalyzed processes;
- From mechanistic studies to design of advanced catalyst systems.

The Conference is accompanied by the School-Symposium of young scientists "Quantum-mechanical modeling of catalytic processes".

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Oxidative Conversion of Light Alkanes for Catalytic Synthesis of Hydrogen

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At present, changes in the structure of production and consumption of hydrocarbons show a steady increase in the role of natural gas as energy and raw materials. The two most important reasons demonstrate this fact:

- significant reserves of natural gas, which are significantly higher than the oil reserves;
- more higher ecological safety of gaseous hydrocarbons.

One-, two- or multicomponent catalysts based on metals of the III and VI groups as well as elements of the I and VIII groups supported on natural and synthetic carriers have been developed to rational selection of catalysts. The developed compositions of catalysts were prepared by incipient wetness impregnation the mixed aqueous solutions of nitrate salts, supported on natural and synthetic carriers, followed by drying at T = 473 K for 2 h. Calcination of the samples at T = 773 K for 2 h in air was carried out for decomposition of supported metal salts and volatilization of nitrates from the catalyst surface.

Activity of developed catalysts was investigated in catalytic oxidation of the C_1 and C_3-C_4 alkanes into hydrogen. Studies on the effect of varying the process parameters and composition of reaction mixture on oxidative conversion of alkanes were carried out.

Oxidative conversion of the methane of natural gas into hydrogen at reaction temperatures varying from 700 to 900°C on the catalysts Ni/ZSM-5+Al_2O_3, Ni-K/ZSM-5+Al_2O_3, Ni-La/ZSM-5+Al_2O_3, Cu-La/ZSM-5+Al_2O_3 and Ni-Cu-Nd/ZSM-5+Al_2O_3 have been studied. It was found that T = 750-900°C and GHSV = 6000 h^{-1} are the optimum conditions for obtaining of 65-69 % hydrogen in the conversion of methane at CH_4 : O_2 : Ar = 7.0 : 1.0 : 92.0 (36.0 : 5.0 : 59.0 %) on the developed bimetallic 5.0 % Cu-La/ZSM-5 + Al_2O_3 catalyst.

Three-component supported 1 % MoCrGa catalyst is most suitable catalyst composition for oxidative conversion of C_3-C_4 mixture in hydrogen at C_3-C_4 : O_2 : N_2 : Ar = 0.95 : 1 : 3.76 : 0.95, T = 550°C, GHSV = 3150 h^{-1}. 70 % hydrogen was obtained as a result of the tests.

Thus, supported mono-, bi- and multicomponent catalysts for oxidation of light alkanes into hydrogen have been developed. It was determined that the three- and bimetallic catalyst systems are optimal for the conversion of initial reaction mixture into hydrogen.

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