BCAS Vol.28 No.3 2014

Promising New Catalyst for Activation and Conversion of Methane Developed at DICP

the large reserves of natural gas around the world, such as shale gas, methane hydrate, and biogas, research on how to utilize these alternative fuels has grown considerably. Current industrial-scale processes for the conversion of natural gases to useful chemical feedstocks, which involves the conversion to syngas intermediates, are complex, inefficient and costly, and they generate large quantities of CO₂ and coke byproducts.

The efficient conversion of these natural gas fuels will require a process wherein the C-H bond of methane is activated, and the methane is selectively converted to useful chemical products while minimizing depth dehydrogenation and overoxidation. Many methods have been developed for the activation and conversion of methane with varying degrees of success, but thus far, none has been viable as industrial-scale processes. The efficient activation and conversion of methane at the industrial-scale thus remains an important challenge in energy research.

A team at Dalian Institute of Chemical Physics led by Prof. BAO Xinhe has recently developed a promising new catalysis that gives a high conversion rate of methane to ethylene, aromatics (benzene and naphthalene), and hydrogen under non-oxidative conditions. The results from their work were presented in the May 9th issue of *Science* (Science 2014, 344, 616-619). Through use of a new catalyst, which consists of lattice-confined single iron sites embedded within a silicide matrix, methane is converted to methyl radicals. The methyl radicals then undergo a series of gas-phase reactions to form products. With this catalyst, a single pass conversion of methane reached 48.1%, and the total selectivity to ethylene and aromatics exceeded 99%, with the selectivity to ethylene reaching 48.4%. This method developed by BAO et al. avoids the energyintensive syngas generation of conventional natural gas



The single iron site confined in a silica lattice enables direct, nonoxidative conversion of methane, exclusively to ethylene and aromatics. The reaction is initiated by catalytic generation of methyl radicals, followed by a series of gas-phase reactions. The absence of adjacent iron sites prevents catalytic C-C coupling, further oligomerization, and hence, coke deposition. (Image by GUO Xiaoguang)

processing. Furthermore, the method leads to little-to-no emission of CO_2 and coke.

The research effort by BAO *et al.* described in the most recent issue of *Science* involved a series of *in situ* experiments at the Shanghai Synchrontron Radiation Facilities, highresolution transmission electron microscopy (HRTEM), and density functional theory (DFT) simulations, which together allowed for the elucidation of the catalyst structure and insights into the underlying reaction mechanism.

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