

Single iron sites for catalytic, nonoxidative conversion of methane

The availability of inexpensive natural gas from the fracturing of shale and as a byproduct of oil production has stimulated the investigation of catalytic processes for the direct conversion of methane to products. Efforts in this direction are further driven by the desire to avoid the generation of CO₂ and its emission to the atmosphere, as occurs when methane is steam-reformed to produce synthesis gas, a mixture of CO and H₂ that can be used for the production of fuels and chemicals via Fischer-Tropsch synthesis. During the past forty years, numerous investigators have attempted to convert methane to higher value products by either thermal dehydrogenation or by oxidative dehydrogenation. While methane can be converted to benzene and hydrogen via thermal dehydrogenation, this process is accompanied by the deposition of large amounts of coke, leading to rapid catalyst deactivation. The oxidative coupling of methane has focused on the formation of ethylene, but this chemistry is not selective and also results in a substantial combustion of methane to CO₂ and water.

In a remarkable new development recently published in *Science* [1], Prof. Xinhe Bao and his collaborators at the Dalian Institute of Chemical Physics and other institutes/universities have succeeded in developing a single-site iron silicide catalyst contained in a silica matrix that is able to convert methane non-oxidatively to ethylene and aromatics virtually quantitatively (Figure 1). While the catalyst requires a very high operating temperature, 1090 °C, it has been found to be stable for 60 h. Methane conversion keeps at 48.1% and ethylene selectivity at 48.4%, whereas the total selectivity to the three products (ethylene, benzene and naphthalene) exceeds 99%. Careful analytical studies conducted using TEM and X-ray absorption spectroscopy, complemented by quantum chemical studies, have demonstrated that isolation of the catalytically active iron sites is

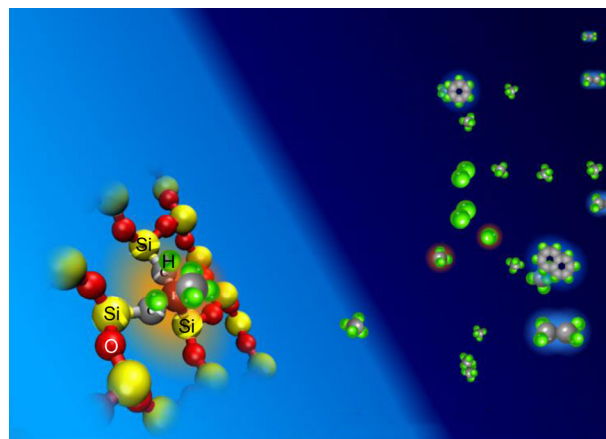


Figure 1 Methane to ethylene over the lattice-confined single iron site.

essential for maintaining catalyst activity and the long term stability. The reaction is initiated by catalytic generation of methyl radicals over these sites, 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. The report by Prof. Bao *et al.* represents an exciting new step forward in the area of direct methane conversion, which is likely to find significant interest in industry.

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- 1 Guo XG, Fang GZ, Li G, Ma H, Fan HJ, Yu L, Ma C, Wu X, Deng DH, Wei MM, Tan DL, Si R, Zhang S, Li JQ, Sun LT, Tang ZC, Pan XL, Bao XH. Direct, nonoxidative conversion of methane to ethylene, aromatics, and hydrogen. *Science*, 2014, 344: 616–619