

# Researchers identify possible catalyst for converting methane to methanol at room temperature

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Ball and stick model of methane. Credit: Ben Mills/Public Domain

(Phys.org)—A team of researchers from Belgium and the U.S. has identified the active site of an iron-containing catalyst that has raised hopes for designing a practically useful catalyst that might make converting methane to methanol a possibility. In their paper published in the journal *Nature*, the researchers describe their efforts, what they discovered and why they believe their findings may lead to a practical way to convert methane to a more efficient energy resource. Jay Labinger, with the California Institute of Technology offers a *News & Views* [piece](#) outlining the work done by the team in the same journal

issue.

Scientists would very much like to find a way to convert [methane](#) (the primary component in natural gas) to methanol at room temperature. Doing so would offer a new source of liquid fuel that would be readily available due to the abundance of methane. Unfortunately, researchers have found it difficult going due to the unreactive nature of methane. In this new effort, the researchers report on progress they believe they have made in achieving that goal.

As Labinger reports, that progress has come in two forms. The first was developing an aid for picking out the [active site](#) of a heterogeneous catalyst from a host of candidates. The second involved creating a design for converting methane to ethanol that would be both efficient and achievable at room temperature.

To create their design, the team looked at an iron-containing structure generated via a zeolite (a type of mineral) that had been reported back in 1997. Since that time, researchers have used various techniques to ascertain that such structures contain another structure known as the  $\alpha$ -Fe(ii) center, an important component in converting methane to [methanol](#) at room temperature. The new design involved proposing a means of describing a structure with an unusual monometallic iron center. They then conducted experiments using Mössbauer spectroscopy that indicated they were on the right track, which could lead eventually to finding the catalyst they are seeking.

The finding by the team is good news, Labinger suggests, though he cautions that it is unlikely that the same approach could be used for solving other catalytic problems.

**More information:** Benjamin E. R. Snyder et al. The active site of low-temperature methane hydroxylation in iron-containing zeolites, *Nature*

(2016). [DOI: 10.1038/nature19059](https://doi.org/10.1038/nature19059)

## Abstract

An efficient catalytic process for converting methane into methanol could have far-reaching economic implications. Iron-containing zeolites (microporous aluminosilicate minerals) are noteworthy in this regard, having an outstanding ability to hydroxylate methane rapidly at room temperature to form methanol. Reactivity occurs at an extra-lattice active site called  $\alpha$ -Fe(II), which is activated by nitrous oxide to form the reactive intermediate  $\alpha$ -O; however, despite nearly three decades of research, the nature of the active site and the factors determining its exceptional reactivity are unclear. The main difficulty is that the reactive species— $\alpha$ -Fe(II) and  $\alpha$ -O—are challenging to probe spectroscopically: data from bulk techniques such as X-ray absorption spectroscopy and magnetic susceptibility are complicated by contributions from inactive 'spectator' iron. Here we show that a site-selective spectroscopic method regularly used in bioinorganic chemistry can overcome this problem. Magnetic circular dichroism reveals  $\alpha$ -Fe(II) to be a mononuclear, high-spin, square planar Fe(II) site, while the reactive intermediate,  $\alpha$ -O, is a mononuclear, high-spin Fe(IV)=O species, whose exceptional reactivity derives from a constrained coordination geometry enforced by the zeolite lattice. These findings illustrate the value of our approach to exploring active sites in heterogeneous systems. The results also suggest that using matrix constraints to activate metal sites for function—producing what is known in the context of metalloenzymes as an 'entatic' state—might be a useful way to tune the activity of heterogeneous catalysts.

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