Oxidation of Ethane to Ethanol by N\textsubscript{2}O in a Metal–Organic Framework with Coordinatively Unsaturated Iron(II) Sites

Scientific Achievement

This work highlights the importance of metal-organic frameworks (MOFs) as catalysts and their ability to support isolated terminal iron–oxo moieties.

Significance and Impact

The use of a MOF to support isolated terminal iron–oxo moieties with an unusual $S = 2$ spin state is a currently unexplored yet highly promising area of research.

Research Details

Experimentally, the magnesium-diluted analogue of Fe\textsubscript{2}(dobdc), Fe\textsubscript{0.1}Mg\textsubscript{1.9}(dobdc), is found to oxidize C\textsubscript{2}H\textsubscript{6} to C\textsubscript{2}H\textsubscript{5}OH in the presence of N\textsubscript{2}O by most likely forming a transient, iron(IV)–oxo intermediate. Quantum mechanical calculations indicate the ground spin state of iron(IV)–oxo to be a quintet.

Figure shows the conversion of C\textsubscript{2}H\textsubscript{6} to C\textsubscript{2}H\textsubscript{5}OH occurring on magnesium-diluted Fe\textsubscript{2}(dobdc) ($d\text{obdc}^{4−} = 2,5$-dioxido-1,4-benzenedicarboxylate), via the formation of Fe(IV)=O intermediate.

[Color code: Fe=orange, Mg=green, O=red, N=dark blue, C=gray, H=light blue]

This work was performed as part of a collaboration between the University of Minnesota and the University of California, Berkeley

Xiao et al. Nature Chemistry (2014) DOI: 10.1038/nchem.1956