

Oxidation of Ethane to Ethanol by N₂O 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 Fe₂(dobdc), Fe_{0.1}Mg_{1.9}(dobdc), is found to oxidize C₂H₆ to C₂H₅OH in the presence of N₂O 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.

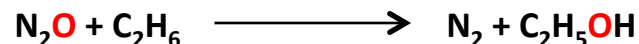
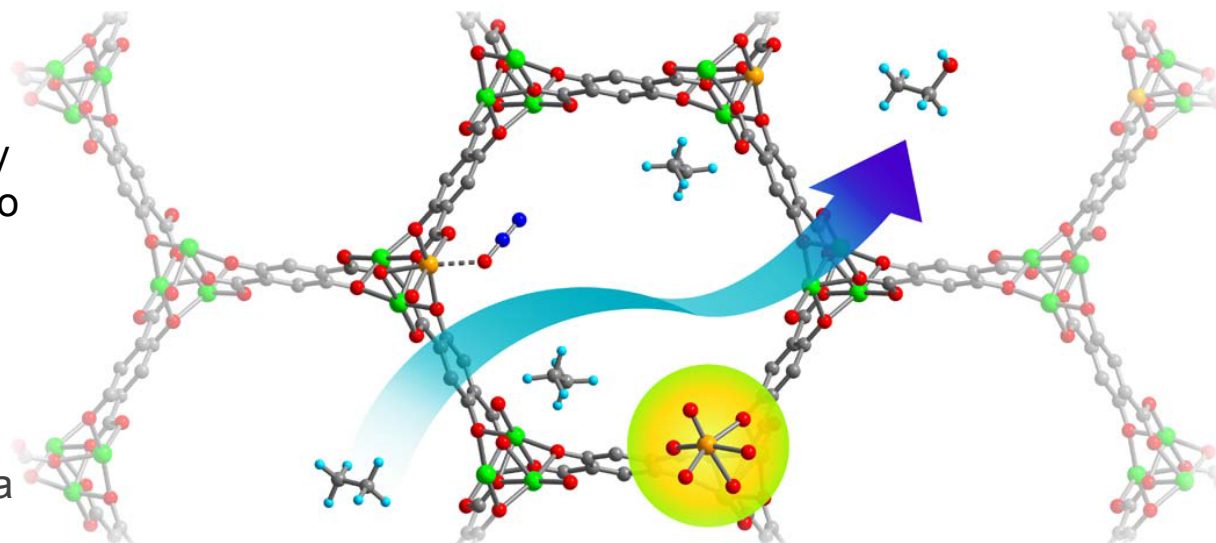


Figure shows the conversion of C₂H₆ to C₂H₅OH occurring on magnesium-diluted Fe₂(dobdc) (dobdc⁴⁻ = 2,5-dioxido-1,4-benzenedicarboxylate), via the formation of Fe(IV)=O intermediate.

[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

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