# *Reactive high-spin iron(IV)-oxo sites through dioxygen activation in a metal–organic framework*


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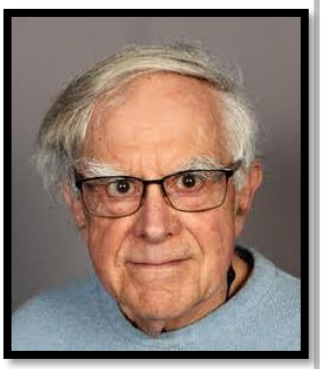

**Chemistry Seminar on *Dioxygen activation by MOF***

**Monday March 9 at 4 pm in 126 Schrenk**

**Please contact Dr. Amitava Choudhury at choudhurya@mst.edu for further information.**

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**Abstract**: The 2025 Nobel Prize in Chemistry was awarded to Richard Robson, Susumu Kitagawa, and Omar Yaghi for groundbreaking work on metal-organic frameworks. These highly porous crystalline frameworks are assembled from metal containing blocks, at the corner, and long organic molecules as edges. They have numerous applications, such as gas storage, biosensors, batteries and fuel cell technology, gas separation, synthesis and catalysis, and water harvesting. In this seminar, a synthetic and catalytic application of a metal-organic frameworks is presented.

In nature, nonheme iron-containing enzymes use dioxygen to generate high-spin iron(IV)=O species for a variety of oxygenation reactions. Although scientists have long sought to mimic this reactivity, the enzyme-like activation of $O_2$ to form high-spin iron(IV)=O species had remained an unrealized goal in synthetic chemistry. In this work, a metal–organic framework featuring iron(II) sites with a local structure similar to that in α-ketoglutarate-dependent dioxygenases has been synthesized. This framework reacts with $O_2$ at low temperatures to form high-spin iron(IV)=O species that are characterized using *in situ* diffuse reflectance infrared Fourier transform, *in situ* and variable-applied magnetic field Mössbauer, Fe Kβ x-ray emission, and nuclear resonance vibrational spectroscopies. In the presence of $O_2$, the framework is effective for catalytic oxygenation of cyclohexane and the stoichiometric conversion of ethane to ethanol.



Hou, K., Börgel, J., et al., *Science*, **382**, 547-553 (2023).


**About the speakers:** Fernande Grandjean received a B.S. and a Ph.D. in physics from the University of Liège, Belgium, in 1968 and 1973. She was a Professor of Physics at the University of Liège, Belgium, from 1983 to 2008 and she is an Adjunct Professor of Chemistry in the Department of Chemistry at Missouri University of Science and Technology. She has published 300 papers and chapters, mostly centered on Mössbauer spectroscopy, and has 14,700 citations and an *h*-index of 63.

Gary J. Long received a B.S. in Chemistry from Carnegie-Mellon University in1964 and a Ph.D. in Chemistry from Syracuse University in 1968; he was a Professor of Chemistry for 53 years at UMR/MST and is now an Emeritus Professor of Chemistry. In 2025, Prof. Long was named a Fellow of the American Association for the Advancement of Science (AAAS). He has published 411 papers and 30 book chapters and has ca. 21,000 citations and an *h*-index of 74.

They have recently published a paper on the "Best Practices and Protocols in Mössbauer Spectroscopy", that serves as the basis for the seminars.