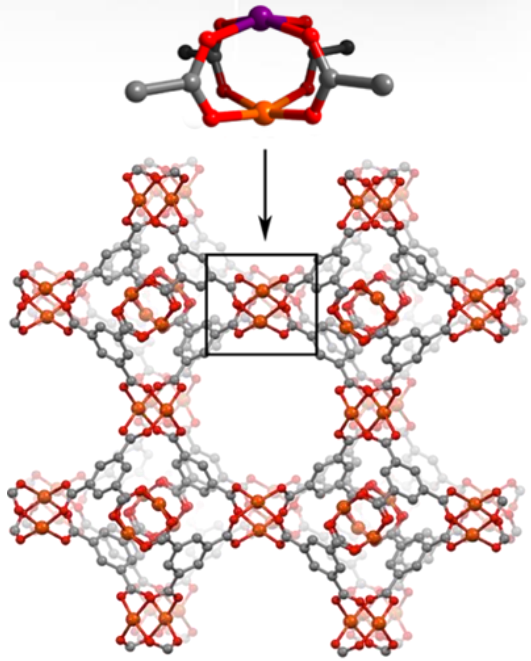
More than just Support: MOFs as Intrinsic Catalysts



The image shows the structure of the crystalline CuRhBTC MOF as well as the bimetallic CuRh node (top).

Scientific Achievement

First study of gas-phase catalytic activity occurring at the nodes of a metal-organic framework (MOF) opens the pathway for tailored active-site geometries in catalysts.

Significance and Impact

MOFs are widely used as a support structure for catalytic reactions; this study uses the MOF itself as a catalyst & allows for unprecedented control of catalyst geometry and active sites.

Research Details

- CuRhBTC MOFs were active & stable for catalytic hydrogenation.
- Density functional theory calculations showed a promising pathway for selective catalysis.
- Multiple characterization techniques confirmed that activity occurs at the Rh(II) ions in the MOF, and the role of Cu is to stabilize the framework.
- NSLS-II QAS beamline provided supporting evidence for the unique Rh(II) oxidation state in the MOF.

D. M. Shakya, O. A. Ejegbavwo, T. Rajeshkumar, S. D. Senanayake, A. J. Brandt, S. Farzandh, N. Acharya, A. M. Ebrahim, A. I. Frenkel, N. Rui, G. L. Tate, J. R. Monnier, K. D. Vogiatzis, N. B. Shustova, D. A. Chen. *Angewandte Chemie* **131**, 16685–16689 (2019).

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