

# Structure of Boron-Based Catalysts from $^{11}\text{B}$ Solid-State NMR at 35.2T

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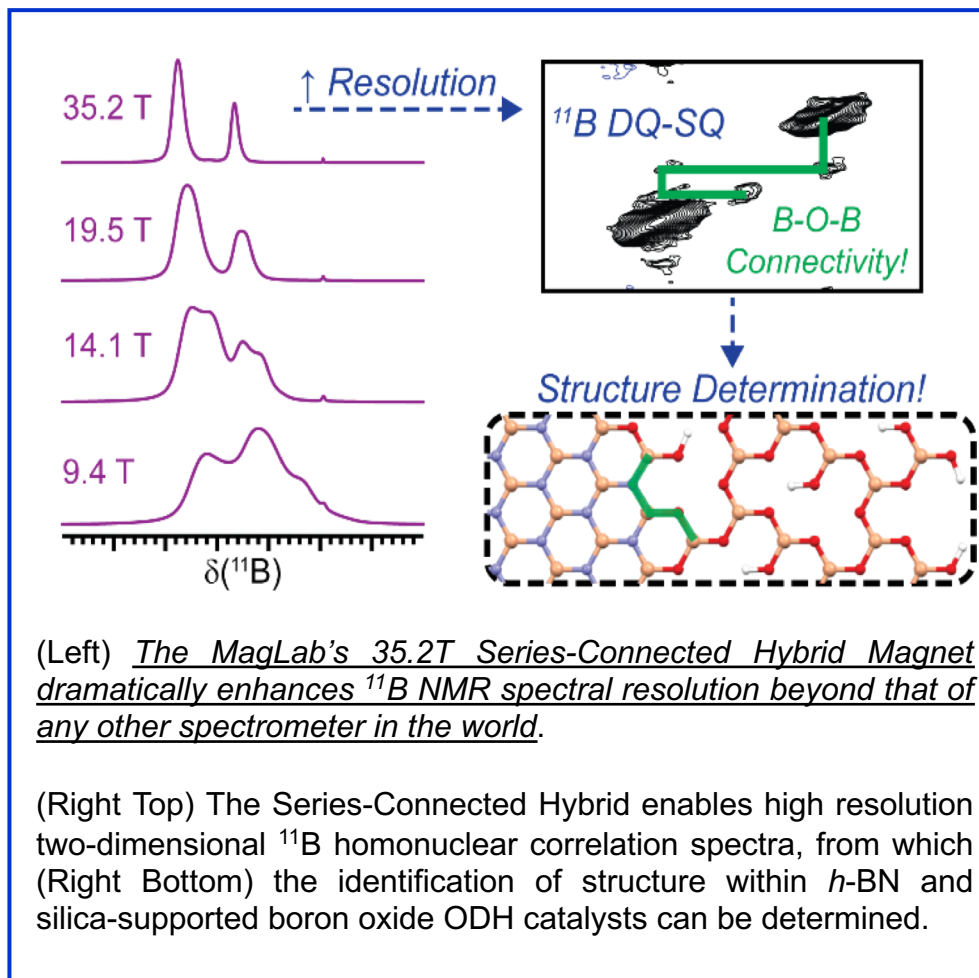
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Boron-based oxidative dehydrogenation catalysts, such as hexagonal boron nitride (*h*-BN) and silica-supported boron oxides, are highly selective catalysts for the oxidative dehydrogenation (ODH) of light alkanes to olefins. Light olefins, such as propylene, are critical chemical feedstocks. The identification of molecular structure of the active sites in catalysts is crucial for the rational design and development of improved ODH catalysts.

MagLab users from Iowa State University and the U.S. DOE Ames Laboratory use high-field solid-state nuclear magnetic resonance (NMR) of boron to characterize boron-based catalysts. Boron-11 ( $^{11}\text{B}$ ) NMR is potentially an ideal technique to determine structure within boron-based materials because it is sensitive to the local chemical environment and the symmetry surrounding the nucleus. However, it can be challenging to identify all of the  $^{11}\text{B}$  NMR signals, because they often overlap due to quadrupolar broadening. The MagLab's 35.2T Series-Connected Hybrid Magnet resolves the  $^{11}\text{B}$  NMR lines, enabling the identification of structure within *h*-BN and silica-supported boron oxide ODH catalysts (featuring only 1wt.% boron) by recording two-dimensional  $^{11}\text{B}$  homonuclear correlation spectra to determine structure in the catalyst. These studies are infeasible in lower-field, conventional NMR magnets.



(Left) The MagLab's 35.2T Series-Connected Hybrid Magnet dramatically enhances  $^{11}\text{B}$  NMR spectral resolution beyond that of any other spectrometer in the world.

(Right Top) The Series-Connected Hybrid enables high resolution two-dimensional  $^{11}\text{B}$  homonuclear correlation spectra, from which (Right Bottom) the identification of structure within *h*-BN and silica-supported boron oxide ODH catalysts can be determined.

**Facilities and instrumentation used:** NMR/MRI, 36T SCH.

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