

## Decoding Structural Complexity of Supported Molecular Catalysts by DNP Surface Enhanced Solid-State NMR Spectroscopy

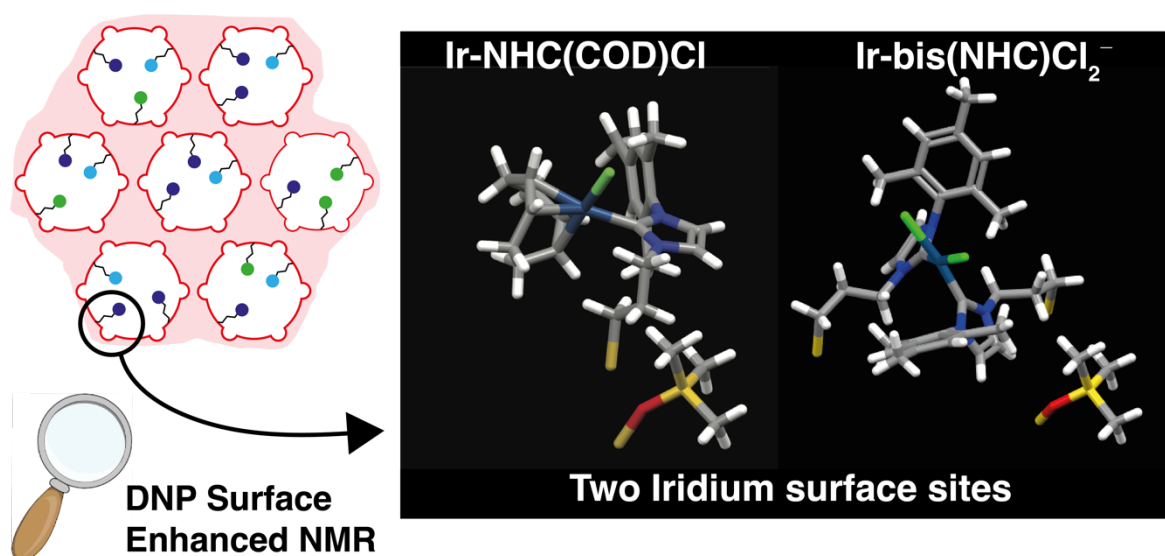
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### ABSTRACT:

Over the last twenty years, solid-state NMR spectroscopy, often in combination with X-ray diffraction techniques, has emerged as a unique analytical method to probe the atomic-scale structure of active sites in heterogeneous catalysts. The recent advent of high-field dynamic nuclear polarization (DNP) has further reinforced the analytic power of solid-state NMR on surfaces (1).

In this presentation we will demonstrate unique methodologies to disclose, with atomic resolution, individual surface structures in complex, multi-site environments, a long-standing challenge in the field of heterogeneous catalysts, while revealing new, unexpected structural features of the supported substrates. These approaches will be illustrated on isolated Ir- N-heterocyclic carbene (NHC) sites (2) as well as on Pt-NHC complexes supported on silica.



**Figure 1:** DNP enhanced solid-state NMR spectroscopy in combination with molecular modeling allows one to elucidate with atomic resolution the 3D structure of the surface sites present in supported molecular catalysts (here the approach revealed two types of Ir-NHC complexes)

### References

- (1) Berruyer, P.; Emsley, L.; Lesage, A. "DNP in Materials Science: Touching the Surface". *eMagRes* **2018**, 7 (4), 93–104.
- (2) Jabbour, R.; Renom-Carrasco, M.; Chan, K.W.; Völker, L.; Berruyer, P.; Wang, W.; Widdifield, C.M.; Lelli, M.; Gajan, D.; Copéret, C.; Thieuleux, C.; Lesage, A. "Multiple Surface Sites Three-Dimensional Structure Determination of a Supported Molecular Catalyst" *J. Am. Chem. Soc.*, doi.org/10.1021/jacs.2c01013