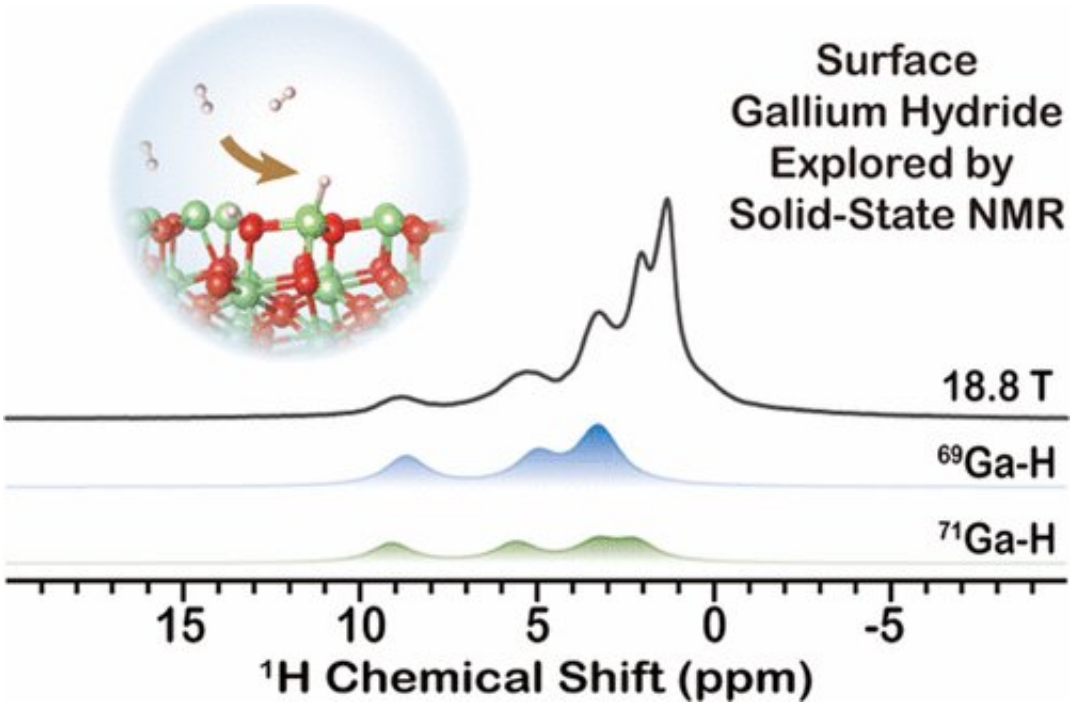
Researchers reveal reactive gallium-hydride species on gallium oxide surface

September 16 2022, by Li Yuan



Graphical abstract. Credit: *Journal of the American Chemical Society* (2022). DOI: 10.1021/jacs.2c01005

Metal hydrides (M-H), critical but ubiquitous intermediates in a broad variety of catalytic reactions, are important in the field of heterogeneous catalysis. However, the comprehensive characterization and understanding of M-H species are still challenging.

Recently, a research team led by Prof. HOU Guangjin from the Dalian

Institute of Chemical Physics (DICP) of the Chinese Academy of Sciences (CAS) revealed the reactive gallium-hydrogen (Ga-H) species on the surface of gallium oxide (Ga_2O_3) by using solid-state nuclear magnetic resonance (ssNMR).

This study was published in *Journal of the American Chemical Society*.

The researchers provided ssNMR evidence of surface Ga-H species generated on a practical nano Ga_2O_3 oxide catalyst during direct H_2 activation and propane dehydrogenation reactions.

They found that the complex ^1H NMR signature of Ga-H species came from strong J and dipolar/quadrupolar couplings using NMR techniques and numerical simulations. And they revealed comprehensive information on the structural configuration and formation mechanism of this special M-H species with complementary NMR and DFT analysis.

Furthermore, they used $^{13}CO_2$ adsorption experiment to prove that Ga-H species were the key intermediates in the hydrogenation process of CO_2.

"The analytic approach presented in this study can be extended to other M–H analysis, and it may benefit the design of more efficient Ga-based catalysts," said Prof. Hou.

More information: Hongyu Chen et al, Direct Detection of Reactive Gallium-Hydride Species on the Ga_2O_3 Surface via Solid-State NMR Spectroscopy, *Journal of the American Chemical Society* (2022). DOI: 10.1021/jacs.2c01005

Provided by Chinese Academy of Sciences