Researchers reveal reactive gallium-hydride species on gallium oxide surface
16 September 2022, by Li Yuan

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.


Provided by Chinese Academy of Sciences

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$_2$O$_3$) 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$_2$O$_3$ oxide catalyst during direct H$_2$ activation and propane dehydrogenation reactions.

They found that the complex $^1$H NMR signature of