'Operando' methods for understanding catalysis in hydrogen storage

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As researchers at Pacifi c Northwest National Laboratory investigated the hydrogen storage capabilities of amine borane compounds, they knew that a rhodium catalyst readily releases hydrogen from the compound at room temperature. But they weren't sure how it worked. Aside from the scientific quest for knowledge, understanding the mechanism at work with rhodium may help with the development of a more cost-effective catalyst to enable hydrogen storage.

PNNL scientists used a type of x-ray spectroscopy available at the Advanced Photon Source synchrotron at Argonne National Laboratory to look at the reaction as it was occurring. They found the active site of the catalyst centered around a cluster of about four rhodium atoms. They also found that the catalyst structure during the reaction was different than the structure before and after the reaction, thus highlighting the importance of measuring the catalyst structure during the reaction conditions.

By combining these results with subsequent in situ nuclear magnetic resonance and infrared spectroscopy, researchers were able to "see" what happens to the boron compound as the hydrogen is released. The results show the mechanism of how the amine borane compound binds to the active catalyst and then how the hydrogen molecule is released as a gas.

The research demonstrates the importance of "operando" methods - or observation of the fundamental molecular level measurements of the catalyst, the reactants and the products - under practical conditions. The

PNNL group is using this approach to investigate other chemical reactions where little is known about the key catalytic processes.