On the way to hydrogen storage?

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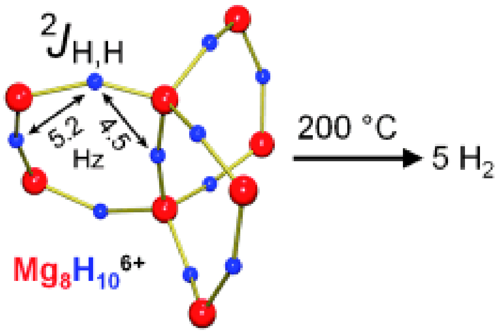

(PhysOrg.com) -- The car of the future could be propelled by a fuel cell powered with hydrogen. But what will the fuel tank look like? Hydrogen gas is not only explosive but also very space-consuming. Storage in the form of very dense solid metal hydrides is a particularly safe alternative that accommodates the gas in a manageable volume. As the storage tank should also not be too heavy and expensive, solid-state chemists worldwide focus on hydrides containing light and abundant metals like magnesium.

Sjoerd Harder and his co-workers at the Universities of Groningen (Netherlands) and Duisburg-Essen (Germany) now take the molecular approach. As the researchers report in the journal *Angewandte Chemie*, extremely small clusters of molecular magnesium hydride could be a useful model substance for more precise studies about the processes involved in hydrogen storage.

Magnesium hydride (MgH_2) can release hydrogen when needed and the resulting magnesium metal reacts back again to form the hydride by pressurizing with hydrogen at a "gas station". Unfortunately, this is an idealized picture. Not only is the speed of hydrogen release/uptake excessively slow (kinetics) but it also only operates at higher temperatures (thermodynamics). The hydrides, the negatively charged hydrogen atoms ($^{H^-}$), are bound so strongly in the crystal lattice of magnesium cations (Mg^{2+}) that temperatures of more than 300 ˚C are needed to release the hydrogen gas.

Particularly intensive milling has made it possible to obtain nanocrystalline materials, which, on account of its larger surface, rapidly release or take up hydrogen. However, the high stability of the magnesium hydride still translates to rather high release temperatures. According to recent computer calculations, magnesium hydride clusters of only a few atoms possibly could generate hydrogen at temperatures far below 300 °C. Clusters with less than 20 Mg^{2+} ions are smaller than one nanometer and behave differently from the bulk material. Their hydride ions have fewer Mg^{2+} neighbors and are more weakly bound. However, it is extremely difficult to obtain such tiny clusters by milling. In Harder's "bottom-up" approach, magnesium hydride clusters are made by starting from molecules. The challenge is to prevent such clusters from forming very stable bulk material. Using a special ligand system, they could trap a cluster that resembles a paddle wheel made of eight Mg^{2+} and ten H^- ions. For the first time it was shown that molecular clusters indeed release hydrogen already at the temperature of 200 °C.

This largest magnesium hydride cluster reported to date is not practical for efficient hydrogen storage but shines new light on a current problem. It is easily studied by molecular methods and as a model system could provide detailed insights in hydrogen storage.

More information: Sjoerd Harder, Hydrogen Storage in Magnesium

Hydride: The Molecular Approach, *Angewandte Chemie International Edition* 2011, 50, No. 18, 4156–4160, dx.doi.org/10.1002/anie.201101153

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