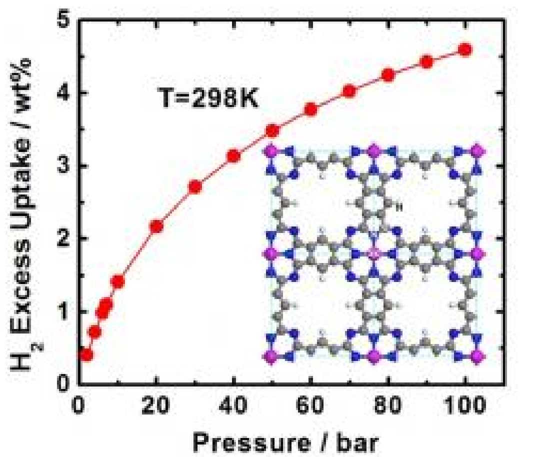
Researchers discover promising hydrogen storage material

November 1 2011, by Lisa Zyga



At a temperature of 298 K and pressure of 100 bar, the new hydrogen material can store hydrogen at a density of 4.6 wt. %. The inset shows the geometry of a Sc-Pc sheet. Image credit: Kun Lü, et al.

(PhysOrg.com) -- If hydrogen is to ever to serve as an onboard energy carrier for the transportation industry, a material will be needed that can store large amounts of hydrogen at ambient temperature and pressure. So far, researchers have not found any material that can meet these requirements. But in a new study, a team from China and the US has taken a significant step toward this goal by identifying a material that can store hydrogen with a density as high as 4.6 wt. % (i.e., the hydrogen accounts for 4.6% of the total weight of the storage material), enabling it to meet the target of 4.3 wt. % set by the US department of Energy for

2010.

The researchers, led by Qiang Sun from Peking University in Beijing, China, and Virginia Commonwealth University in the Richmond, Virginia, US, have published their study in a recent issue of Applied Physics Letters.

"Hydrogen storage is a big challenge for the hydrogen economy," Sun told *PhysOrg.com*. "Currently the research is behind schedule, but with the advancement of materials design and synthesis, reaching the target for future transportation applications [is becoming] more and more promising."

As the researchers explained, the greatest difficulty in finding a sufficient hydrogen storage material for onboard storage systems lies in meeting multiple requirements with a single material. For example, in previous studies researchers have found that light metal hydrides can store hydrogen with a gravimetric density of 20 wt. %, but the material is not reversible, meaning it cannot be reused. Also, the hydrogen desorbs only at very high temperatures. In contrast, other materials such as carbon nanotubes and metal or covalent organic frameworks can store hydrogen reversibly, but the hydrogen adsorbs only at very low temperatures. The difference is due to bonding: in light metal hydrides, hydrogen is held in much stronger bonds than in the second group of materials. The researchers explain that, ideally, hydrogen should be bound with an intermediate binding energy.

"If the bonding is too strong, hydrogen can only be released at high temperature, while if the bonding is too weak, the storage is unstable at room temperature," Sun explained. "So we require an intermediate bonding energy."

In the current study, the researchers used modeling and simulations to investigate the performance of hydrogen storage in metal-containing porous sheets, which can be synthesized using the techniques previously proposed by two other groups (M. Abel, et al., and A. Sperl, et al.). In those techniques, porous sheets were made of blue-green dye units called phthalocyanines (Pc) with regularly spaced iron (Fe) atoms or other metal atoms. Due to their high dispersion, these metal sites in the porous substrates provide the possible adsorption sites for hydrogen molecules.

"Transition metal atoms easily aggregate to form clusters," Sun said. But materials in which metal atoms can be prevented from coalescing are scarce.

The researchers systematically investigated 10 Pc-based porous sheets with transition metal atoms from scandium (Sc) through zinc (Zn), and found that porous Pc sheets with Sc atoms could store up to 4.6 wt. % hydrogen. In addition to the Sc atoms' regular distribution in the Pc sheet, Sc has two other attractive features. First, it is lighter than other transition elements, allowing the overall storage material to be relatively light. Second, Sc atoms have a large size, so that they stick out and can capture more hydrogen molecules.

By theoretically demonstrating that this Sc-Pc porous sheet can be used to create a hydrogen storage material with attractive properties, the researchers hope that the results will stimulate further analysis and experimental tests of the promising material.

More information: Kun Lü, et al. "Sc-phthalocyanine sheet: Promising material for hydrogen storage." *Applied Physics Letters* 99, 163104 (2011). DOI:10.1063/1.3653465