

A promising step towards more effective hydrogen storage

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An international research team led by Swedish Professor Rajeev Ahuja, Uppsala University, has demonstrated an atomistic mechanism of hydrogen release in magnesium nanoparticles – a potential hydrogen storage material. The findings have been published in the online edition of *Proceedings of the National Academy of Science (PNAS)*.

It is becoming clear that cars of the future will have to move from using the combination of petrol and a combustion engine in order to combat global warming and potential oil shortages.

One of the prime candidate technologies are fuel cells using hydrogen gas as fuel, chiefly because hydrogen is among the most abundant elements on earth and is able of producing energy through chemical reactions with oxygen in the fuel cells releasing only water - an environmentally benign by-product. Storing hydrogen gas in a compact way is, however, still an unsolved problem.

Much research effort has been directed at absorbing hydrogen in metal powders, forming so-called metal hydrides. Magnesium may absorb up to 7.7 weight per cent of hydrogen, and has commonly been studied for this purpose, especially since fast loading and unloading of hydrogen can be accomplished by adding catalysts like iron and nickel particles.

It has been speculated that the catalysts act as shuttles, helping to transport hydrogen out of the material. With the help of computer simulations of magnesium clusters at the quantum mechanical level, the

Uppsala researchers and their colleagues have now been able to show in atomic scale how this happens and why only a small amount of catalysts are necessary to improve the hydrogen release. The extensive simulations were performed at Uppsala University's Multidisciplinary Center for Advanced Computational Science (UPPMAX).

"We expect the findings to aid further technical improvements of magnesium-based hydrogen storage materials, as well as other related light metal hydrides," says Professor Raajev Ahuja.

Source: Uppsala University

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