Buckyballs, nanotubes show promise

Gaithersburg, MD, and Golden, CO: Two research groups have independently reported a new take on hydrogen storage with the publication of computational-modelling studies that predict a storage potential of as much as 9 wt% for Buckminsterfullerene (C60) and carbon nanotube molecules "decorated" with light transition metals. Coincidentally, both groups - one a collaboration between the National Institute of Standards and Technology (NIST) in Gaithersburg, Maryland, and Bilkent University, Ankara, Turkey; the other from the National Renewable Energy Laboratory, Golden, Colorado, US - published their findings within days of each other in the journal Physical Review Letters.

NREL's calculations show that a particular scandium (Sc) organometallic "buckyball" (C48B12Sc12H12) could bind as many as five additional hydrogen molecules per Sc atom (Y Zhou et al. 2005 PRL 94 175 504). In the model, Sc bonds to the 12 pentagonal faces of C60. The hydrogen storage potential of this structure is approaching 9 wt%; furthermore, the binding energy of the H2-Sc interaction is calculated to be about 0.4 eV per hydrogen molecule - a perfect match to the adsorption/desorption characteristics required for on-board storage of hydrogen in vehicle applications.

The bonding mechanism observed is described as "Dewar coordination to bind transition metals to carbon rings and a Kubas interaction to bind oligohydrogen species". The NIST-Bilkent group chose to start with carbon nanotubes (T Yildirim and S Ciraci 2005 PRL 94 155 501). In its model, transition metals are shown bonding to hexagonal faces. The researchers found that a single titanium (Ti) atom adsorbed on the nanotube walls can contain, for example, titanium through a unique hybridization between Ti-4d, hydrogen s* antibonding and nanotube C-p orbitals, essentially similar to the Dewar model.

"Both sides were shocked when we saw each others' papers in PRL [Physical Review Letters]," said Taner Yildirim of NIST. The shock was probably particularly heartfelt by the NIST-Bilkent team, which submitted its paper a few weeks before the NREL team only to see it appear two weeks after the NREL findings.

The competition between the two groups is evident, but in this case it certainly appears to be constructive. NREL's Shanghai Zhang told The Fuel Cell Review: "The fact that these two papers emerged independently and essentially simultaneously, with similar results, despite the approach and method being different, indicates the robustness of the idea." Yildirim echoed the sentiment: "I think the fact that two independent groups come up with a very similar idea is an interesting coincidence and a clear indication that we are finally on the right track."

Both teams are also involved in related experimental work. Of the NIST-Bilkent work, Yildirim added: "We are confident that soon we will experimentally confirm the unusual hydrogen bonding that we predict." Meanwhile, NREL's Michael Heben believes that "as the production costs for nanostructured carbon materials come down, these hybrid materials may soon be inexpensively available in the future".

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