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Hydrogen Storage in Novel Carbon-based Nanostructured Materials ERIN WHITNEY, CALVIN CURTIS, CHAIWAT ENGTRAKUL, MARK DAVIS, KIM JONES, PHILIP PARILLA, LIN SIMPSON, ANNE DILLON, NREL, NREL TEAM — One of the biggest challenges facing a future hydrogen economy is that of onboard vehicular hydrogen storage, for which novel carbon-based nanostructured materials have emerged as potential candidates. Towards this end, we present the synthesis and characterization of "bucky dumbbell," a new organometallic compound comprised of two buckyballs complexed to a central iron atom. This new compound has been characterized using both ^{13}C solid-state NMR and Raman spectroscopy, and electron spin paramagnetic resonance spectroscopy reveals the presence of Fe^{3+}. Temperature-programmed desorption has revealed a new hydrogen binding site via the appearance of a peak centered at approximately -50 $^{\circ}$C, indicating the hydrogen is stabilized at a temperature significantly above that expected for physisorption but still lower than that of C-H bond formation. Comparison with C_{60} under the same hydrogen exposure and heating conditions shows almost no hydrogen adsorption, and the exact binding energy (or desorption activation energy, E_d) for the bucky dumbbell shows an enhanced value of $\sim$6.2 kJ/mol. Initial volumetric analyses conducted at 77K and 3 bar show a storage capacity of $\sim$0.4 wt%. The synthesis and analysis of other novel fullerene-based organometallic hydrogen complexes will also be discussed.

Erin Whitney
NREL

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