Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Endohedral Metallofullerenes: A Smart Material for Hydrogen Storage YUFENG ZHAO, MICHAEL J. HEBEN, ANNE C. DILLON, LIN SIMPSON, JEFF BLACKBURN, National Renewable Energy Lab., HARRY C. DORN, Virginia Polytechnic Institute and State University, SHENGBAI B. ZHANG, National Renewable Energy Lab. — We report a first-principle computational study on tunable hydrogenation of the fullerene C_{60} and endohedral metallofullerenes M@C_{60} and M_2@C_{60} (M = Li, Be, Mg, Ca, Al, and Sc). The interaction between the encapsulated metal atoms and the C_{60} cage leads to a smart-material behavior, which tunes the hydrogen binding in a desired manner as the hydrogenation proceeds. At lower H densities, when H atoms are too strongly bound to pure C_{60}, the endohedral dopants weaken the binding. The dopants also enhance the hydrogen binding energy at higher coverages, and enable the degree of hydrogenation to be substantially increased relative to that available with un-modified C_{60}. Overall, the encapsulated metals increase the capacity and improve the energy efficiency for hydrogen storage in hydroendofullerides.

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Date submitted: 20 Nov 2006 Electronic form version 1.4