

Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Hydrogen storage on calcium coated boron (hetero-)fullerenes: A DFT study SULEYMAN ER, Harvard University, GEERT BROCKS, University of Twente, GILLES A. DE WIJS, Radboud University Nijmegen — Using density functional theory (DFT), we investigate hydrogen storage properties of calcium-coated molecular systems of B₈₀ boron fullerene, C₄₈B₁₂ boron-doped heterofullerenes, and well-known C₆₀ fullerene. Here, we consider the most common and low-lying isomers of B₈₀ and C₄₈B₁₂. We find that the Ca-coated molecules have the following properties: (1) The binding of metal atoms to B₈₀ or to C₄₈B₁₂ molecules is much stronger than their binding to a C₆₀ molecule. (2) B₈₀ and C₄₈B₁₂ have larger electron affinities than their carbon only counterpart, and accordingly discharge the surface Ca atoms more efficiently. (3) B₈₀ molecule, however, shows structural deformations upon reacting with Ca atoms. (4) C₄₈B₁₂Ca₆, however, is stable at elevated temperatures. C₄₈B₁₂ has well-exposed, positively charged Ca atoms on its surface, and binds up to six hydrogen molecules per metal center with hydrogen binding energies of 0.17-0.14 eV/H₂, that are suitable for ambient temperature hydrogen storage.

Suleyman Er
Harvard University

Date submitted: 19 Dec 2011

Electronic form version 1.4