

Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Hydrogen Storage in Titanium-decorated Boron Buckyball JIA LI, GANG ZHOU, WENHUI DUAN, Department of Physics, Tsinghua University, Beijing 100084, PR China, HOONKYUNG LEE, JISOON IHM, Department of Physics and Astronomy, Seoul 151-747, Korea — Using first-principles electronic structure calculations, we investigate the potential of Ti-decorated B₈₀ for hydrogen storage medium. The Ti-decorated B₈₀ has the merit of an unexpected large binding energy of a Ti atom to B₈₀ which can overcome the problem of metal clustering. Up to four hydrogen molecules are found to be adsorbed on a single Ti atom coated on B₈₀. At high Ti coverage, we show that the Ti-decorated B₈₀ can adsorb up to 5 wt% hydrogen and the calculated binding energy falls in the desirable range of 0.2-0.6eV/H₂ which is suitable for reversible hydrogen storage at room-temperature, near-ambient-pressure conditions.

Jia Li
Department of Physics, Tsinghua University, Beijing 100084, PR China

Date submitted: 12 Nov 2007

Electronic form version 1.4