Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Hydrogen storage in BN cage PURU JENA, QIANG SUN, QIAN WANG, Virginia Commonwealth University — Recently hydrogen is being considered as a potential candidate to meet the increasing energy need of both the developing and developed world. To this end it is important to find efficient means for storing hydrogen. Carbon nanotubes, especially single-wall tubes, were initially considered to be better candidates for hydrogen storage than other materials. However, the early experiments have met with some controversy and very different results for the hydrogen storing capacity of carbon nano-tubes have been reported. To search for other non-carbon system, we studied $(H_2)_n@B_{36}N_{36}$ cage by using first-principles method. It has been found that H_2 can go into the cage through the hexagonal face. The maximum number of H_2 that can be inserted into the cage without breaking the cage is 18, resulting in a weight percentage of 4%. However, the storage of H_2 in BN cage needs external energy, which increases with n^2 (n is the number of hydrogen molecules) while the HOMO-LUMO gap decreases as n^3. The energy cost is associated with the increase in the B-N bond length and decrease in the H-H bond length as n increases.

Puru Jena
Virginia Commonwealth University

Date submitted: 22 Nov 2004 Electronic form version 1.4