Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Hydrogen storage in ammonia borane: *Ab initio* **study of the de- and rehydrogenation mechanisms**[1] KISEOK CHANG, DAVID TOMÁNEK, Michigan State University, EUNJA KIM, PHILIPPE F. WECK, University of Nevada Las Vegas — Using *ab initio* density functional calculations, we study the microscopic mechanism of hydrogen release from ammonia borane (NH_3BH_3) and the reverse process leading to its subsequent recharging with hydrogen. Our total energy surfaces indicate the most favorable pathways to thermally convert the NH_3BH_3 molecular solid to the energetically preferred polymer NH_2BH_2 and molecular hydrogen. To prevent formation of undesirable side-products such as the cyclic compound borazine ($N_3B_3H_6$) or other complexes that would prevent subsequent rehydrogenation, we propose to enclose AB in narrow carbon nanotubes. In this constrained space, we investigate possible rehydrogenation pathways using atomic and molecular hydrogen as well as selected protonation agents.

[1]Supported by NSF NSEC Grant 425826 and NSF-NIRT grant ECS- 0506309.

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Date submitted: 20 Nov 2008 Electronic form version 1.4