

Abstract Submitted  
for the MAR09 Meeting of  
The American Physical Society

**Cubic Metallic Phase of Aluminum Hydride Showing Improved Hydrogen Desorption** RALPH H. SCHEICHER, DUCK YOUNG KIM, Condensed Matter Theory Group, Department of Physics and Materials Science, Uppsala University, Uppsala, Sweden, RAJEEV AHUJA, CMT Group, Uppsala Univ.; Applied Materials Physics, Department of Materials and Engineering, Royal Institute of Technology (KTH), Stockholm, Sweden — AlH<sub>3</sub> is of great interest for hydrogen storage applications, with a particularly attractive feature being its large hydrogen capacity of 10 wt.%. Here we report the results of our density functional theory study of the dehydrogenation properties in a cubic phase of AlH<sub>3</sub>. The metallic nature of the electronic structure entails a more favorable hydrogen removal energy which is lowered by 75% compared to the insulating hexagonal phase. This remarkable reduction in the Al–H bond strength might bear important consequences for feasible applications of AlH<sub>3</sub> as an on-board hydrogen storage material for mobile applications. Suggestions are made how the cubic phase could be prepared and stabilized at ambient pressure by off-board quenching. See also: R. H. Scheicher, D. Y. Kim, S. Lebègue, B. Arnaud, M. Alouani, and R. Ahuja, *Appl. Phys. Lett.* **92**, 201903 (2008) and D. Y. Kim, R. H. Scheicher, and R. Ahuja, *Phys. Rev. B* **78**, 100102(R) (2008).

Ralph H. Scheicher

Date submitted: 17 Nov 2008

Electronic form version 1.4