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$_3$ 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$_3$. 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$_3$ 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