

Abstract Submitted  
for the MAR11 Meeting of  
The American Physical Society

**Ultra-low diffusion barriers for the  $\text{AlH}_3$ -related vacancies in  $\gamma$ - $\text{NaAlH}_4$**  FENG ZHANG, YAN WANG, MEI-YIN CHOU, School of Physics, Georgia Institute of Technology — It has been suggested that the diffusion of  $\text{AlH}_3$ -related vacancies plays an essential role in the decomposition of  $\text{NaAlH}_4$ , a prototypical material for hydrogen storage[1,2]. We find from first-principles calculations that the diffusion barrier for both the neutral  $\text{AlH}_3$  vacancy and the charged  $\text{AlH}_4^-$  vacancy in the newly proposed  $\gamma$ -phase of  $\text{NaAlH}_4$  [3] is only about 0.1 eV, much lower than the barrier for the diffusion of corresponding vacancies in the conventional  $\alpha$ -phase 0.5 eV, calculated with the same method. Possible schemes to facilitate the  $\alpha \rightarrow \gamma$  phase transformation in order to improve the kinetics of the decomposition reaction of  $\text{NaAlH}_4$  will also be discussed.

- [1] H. Gunaydin, K. N. Houk, and V. Ozoliņš, Proc Natl Acad Sci USA **105**, 3673 (2008).
- [2] G. B. Wilson-Short, A. Janotti, K. Hoang, A. Peles, and C. G. Van de Walle, Phys. Rev. B **80**, 224102 (2009).
- [3] B. Wood and N. Marzari, Phys. Rev. Lett. **103**, 185901; **104**, 019901.

Feng Zhang

Date submitted: 28 Dec 2010

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