

Abstract Submitted
for the CAL09 Meeting of
The American Physical Society

Comparative analysis of the hydrogen-vacancy interaction in Mg and Al based on density functional theory¹ LARS ISMER, A. JANOTTI, C.G. VAN DE WALLE, Materials Department, University of California, Santa Barbara, CA 93106-5050 — The interactions of vacancies (V) with atomic hydrogen (H) in the bulk of the metal are expected to play an important role in H-storage as well as H-embrittlement. Using density functional theory we have studied the H-V interactions in hcp-Mg and fcc-Al, two prototypic systems for H storage. We show that a single V can in principle host up to 9 H atoms in Mg and 10 in Al. In going beyond previous theoretical studies we further evaluate the concentration of the H-V complexes for different H loading conditions – ranging from low pressures to high pressures of H₂ gas. We find significant differences between Mg and Al. In the case of Al, up to 15 % of H atoms are trapped in single vacancies even for very low H pressures, which strongly slows down the diffusion of H atoms. In the case of Mg, these trapping effects are negligible for low H pressures. However, vacancies containing multiple H atoms and H-induced superabundant vacancy formation are predicted to occur in Mg at much lower H loading pressures (about 1 GPa) than in Al (about 10 GPa).

¹This work was supported by the U. S. DOE (Grant No. DE-FG02-07ER46434) and made use of the CNSI (NSF Grant No. CHE- 0321368) and the NSF-funded TeraGrid (Grant No. DMR070072N) computers.

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Date submitted: 23 Oct 2009

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