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Tuning the Hydrogen Storage in Magnesium Alloys SULEYMAN ER, University of Twente, GILLES A. DE WIJS, GEERT BROCKS — We investigate the hydrogen storage properties of promising magnesium alloys. MgH_2 (7.6 wt % H) would be a very useful storage material if the (de)hydrogenation kinetics can be improved and the desorption temperature is markedly lowered. Using first principles calculations, we show that hydrides of Mg-transition metal (TM) alloys adopt a structure that promotes faster (de)hydrogenation kinetics, as is also observed in experiment [1]. Within the lightweight TMs, the most promising alloying element is titanium. Alloying Mg with Ti alone, however, is not sufficient to decrease the stability of the hydride phases, which is necessary to reduce the hydrogen desorption temperature [2]. We find that adding aluminium or silicon markedly destabilizes Mg-Ti hydrides and stabilizes Mg-Ti alloys. Finally, we show that controlling the structure of Mg-Ti-Al(Si) system by growing it as multilayers, has a beneficial influence on the thermodynamic properties and makes it a stronger candidate for hydrogen storage [3].

Ref: [1] S. Er *et al.*, Phys. Rev. B, **79**, 024105 (2009). [2] S. Er *et al.*, J. Phys.: Condens. Matter, **22**, 074208 (2010). [3] S. Er *et al.*, J. Phys. Chem. Lett., **1**, 1982 (2010).

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