SUPPORTING INFORMATION PARAGRAPH

Metallic and Carbon Nanotubes-Catalysed Coupling of Hydrogenation in Magnesium

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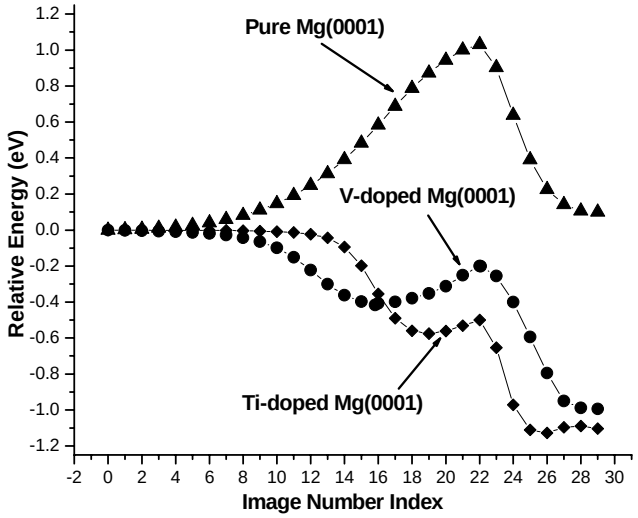

Fig. 1S

Supporting information: Hydrogen dissociation at the Mg(0001) surface: energy barriers and associated minimum-energy-pathway profiles for pure Mg, V-incorporated and Ti-incorporated Mg(0001) surfaces.

The energy profile for hydrogen dissociation in the presence of the metallic catalyst (V or Ti) is dramatically altered compared to the pure Mg surface. Firstly, the hydrogen molecule approaches the catalyst atom (which is incorporated in the Mg surface) without any energy barrier. Then, the hydrogen molecule dissociates into two atoms at the Vi or Ti site with a much smaller energy barrier (0.201 and 0.103eV for

V and Ti, respectively) compared to that on a pure Mg surface (1.15eV). Subsequently, the dissociated hydrogen atoms interact with the metallic catalyst (V or Ti) to form V/Ti-H bonds (with an energy reduction of 0.75 and 0.6eV for V and Ti, respectively). Finally, the formed V/Ti-H bonds can be easily rotated around the metallic atom without any energy barrier (V-H bond) or with a very small energy barrier of 0.04eV (Ti-H bond).

Figure 2S HRTEM image of *MgH_2-VTi- CNT*