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Stability of transition metals on the Mg-terminated MgB_2 (0001) surface and their effects on hydrogen dissociation YONGLI WANG, CHRIS WOLVERTON, Northwestern University — The re-hydrogenation of MgB_2 is a critical step in the reversibility of several key hydrogen storage reactions. Two main activated processes affect the kinetics of hydrogen absorption by MgB_2: the dissociation of the H_2 molecule and the diffusion of atomic H into the bulk. In order to have fast absorption kinetics both activated processes need to have a low barrier. Using first-principles calculations, we investigate the dissociation of H_2 on the Mg-terminated MgB_2 (0001) surfaces. We investigate both ideal surfaces as well as surfaces with vacancies, and transition-metal-dopants (TM=Sc∼Zn,Y∼Cd,Au,Pt). Our calculations show that the late TMs more favorably substitute for the Mg atoms in the outermost layer of the Mg-terminated surface, rather than for those in the sub-layers. We find the dissociation barrier for H_2 on the clean Mg-terminated MgB_2 (0001) surface is 0.46eV. The TM dopants have only a small effect on dissociation barrier when they are incorporated into the sub-layers. However, when doped in the outermost layer, we find examples of dopants that significantly decrease the activation barrier for the dissociation of H_2. We also investigate the diffusivity of H in MgB_2 and find strong anisotropy in the diffusion pathways.

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