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Dehydrogenation in catalyst activated MgH_2[1] SA LI, PURU JENA, RAJEEV AHUJA, Virginia Commonwealth University, VIRGINIA COMMONWEALTH UNIVERSITY TEAM, UPPSALA UNIVERSITY COLLABORATION
— Dehydrogenation in catalyst activated magnesium hydride (MgH_2) has been investigated using *ab initio* Molecular Dynamics (MD) simulation and Nudged Elastic Band (NEB) method. Our calculation explains why small amount of Nb_2O_5 catalyst can substantially improve the thermodynamics and kinetics of MgH_2. We show that Nb_2O_5 promotes the creation of Mg vacancies and that the hydrogen desorption from the vicinity of Mg vacancies occurs in molecular form and is exothermic. The activation energy barrier for H_2 desorption in vacancy containing magnesium hydride (1.02 eV) is much lower than that in the pure magnesium hydride (3.30 eV). Therefore, the effective catalyst for dehydrogenation in MgH_2 will be one that can easily facilitate MgO formation.

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