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$_2$O$_5$ catalyst can substantially improve the thermodynamics and kinetics of MgH$_2$. We show that Nb$_2$O$_5$ 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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