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Effect of Ti and metal vacancies on the dehydrogenation of Na_3AlH_6 ¹ SA LI, PURU JENA, Virginia Commonwealth University, RAJEEV AHUJA, Uppsala University, VIRGINIA COMMONWEALTH UNIVERSITY TEAM, UPPSALA UNIVERSITY COLLABORATION — Electronic and structural properties of sodium-aluminum hexahydride (Na_3AlH_6) formed during the decomposition reaction of sodium alanate (NaAlH_4) are calculated using density functional theory and generalized gradient approximation for exchange and correlation potential. The roles of Ti substitution at the Na and Al sites as well as that of Na and Al vacancies on the desorption of hydrogen have also been investigated. We show that the improvement in dehydrogenation of Na_3AlH_6 is due to the addition of Ti much the same way as that in NaAlH_4 , namely through the weakening of the metal-hydrogen bond. However, as in the case of NaAlH_4 , vacancies are found to be more effective in desorbing hydrogen at lower temperatures than Ti substitution at the Na or Al sites.

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