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Ti-based catalytic effect on hydrogen desorption in crystalline NaBH4: an ab initio investigation C. MOYSÉS ARAÚJO, RAJEEV AHUJA, University of Uppsala, PURU JENA, Virginia Commonwealth University — The application of hydrogen fuel cell technology in portable electronic devices and transportation vehicles has led to a great deal of interest in the study of complex alkali hydrides (MXH_4 with M=Na, Li and X=Al,B) primarily due to their high gravimetric hydrogen density (eg.18.5% in $LiBH_4$). In particular, $NaBH_4$ slurry has been suggested as the most promising system for applications in fuel cell technology (1) as it provides one of the simplest ways of generating hydrogen. Additionally, the $NaBH_4$ itself is also a promising hydrogen storage material since it has one of the highest gravimetric hydrogen density (13.0 wt%) among the alkali metal hydrides. However, its irreversibility with respect to hydrogen absorpton/desorption cycle limits its practical application for hydrogen storage. To overcome this limitation we have explored the role of Ti on the electronic and crystalline structures of $NaBH_4$. Using density functional calculations we show that Ti prefers to occupy the Na site in sodium borohydride. In addition, Ti weakens the strength of the covalent bond between B and H atoms and the hydrogen removal energy is reduced from 5.64 eV in pure sodium borohydride to 4.70 eV when doped with Ti. Thus, Ti might work as a catalytic agent allowing hydrogen to desorb at a lower temperature. Calculations are underway to examine if other dopants may be even better candidates for hydrogen desorption from sodium borohydride. 1. Z. P. Li, B. H. Liu, K. Arai, K. Asaba and S. Suda *Journal of Power Sources* **126**, 28 (2004).

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