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Theoretical Analysis on X-ray Absorption Spectra of Ti compounds as Catalysts in Lithium Amide-Imide reactions TAKAO TSUMURAYA, TATSUYA SHISHIDOU, TAMIO OGUCHI, Hiroshima University — Solid-state storage is conceptually efficient approach for on-board vehicular hydrogen storage. In this context, light-element materials such as lithium amide $LiNH_2$ and lithium imide Li_2NH have been attracted much attention due to their high gravimetric densities of hydrogen. Recently, various transition-metal compounds have been examined with ball-milling technique for exploring catalysts to improve the hydrogen storage and desorption kinetics, and it is found that a small amount (1mol%) of titanium compounds revealed a superior effect in hydrogen desorption reaction $LiNH_2 + LiH \rightarrow Li_2NH + H_2$ [1]. However, these catalysis mechanism and role of Ti in the reaction remain unanswered. Isobe *et al.* have carried out measurements of X-ray absorption spectroscopy(XAS) at Ti K-edge to see the electronic states of Ti recently [2]. In this paper, we calculate the electronic structure of Ti metal and its compounds, and obtained theoretical spectra to compare with the measured spectra by using first-principles calculations based on the all-electron FLAPW method. We discuss chemical bonding and local geometry of catalytically active states in the reaction. [1] T. Ichikawa, S. Isobe, N. Hanada and H. Fujii, J. of Alloys and Comp. 365, 271 (2004) . [2] S. Isobe, T. Ichikawa, Y. Kojima and H. Fujii, J. of Alloys and Comp. 446-447, 360 (2007).

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