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Lithium Fast-Ion Conduction in Complex Hydrides

A few years ago, an exceptional high Li mobility was discovered within the high temperature (HT) phase of $LiBH_4$.by IMR scientists [1]. Stabilizing the HT phase by adding lithium halides results in an enhanced conductivity at room temperature [2]. Even higher conductivities are reached by combining BH_4 and NH_2 anions in compounds such as $Li_2(BH_4)(NH_2)$ [3]. We investigated $LiBH_4$ based compounds in view of their potential applications as Li-ion conductors and/or as hydrogen storage materials

Continuous depletion of fossil fuels and growing environmental concerns make energy supply one of the major challenges in the 21st century. The implementation of renewable energy requires new high performance materials for energy conversion, transport and storage. For industrial applications these materials have to be cheap, safe and reliable in their performance. Currently, materials for lithium ion batteries, photovoltaics, fuel cells and electrolyser cells, and materials for hydrogen production and storage are in the focus of many research activities worldwide.

Borohydrides are ionic stable materials that contain light metal cation and BH_4 groups, which are considered as high performance hydrogen storage media. Recently an exceptional high Li mobility was discovered within the high temperature (HT) phase of LiBH4. Stabilization of the HT phase of this compound by addition of lithium halides results in an enhanced conductivity also at room temperature. Even higher conductivities are reached by combining $(BH_4)^-$ and $(NH_2)^-$ anions in compounds such as $Li_2(BH_4)(NH_2)$, as shown in fig.1.

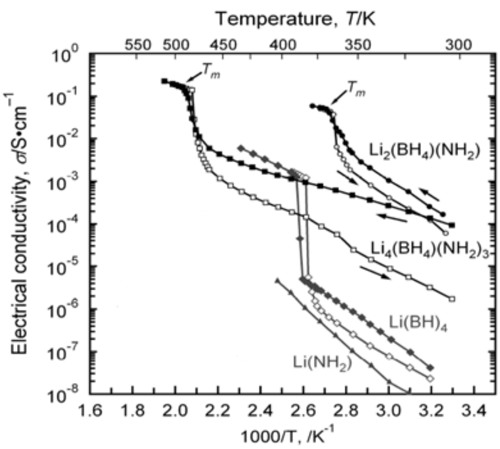

Figure 1: Electrical conductivities of $LiBH_4$, $LiNH_2$, $Li_2(BH_4)(NH_2)$ and $Li_4(BH_4)(NH_2)_3$ (triangle).

Up to now, the origin of the phase transition, and therefore the role of the halides as stabilizing agents are not understood. Also the transport mechanism in borohydrides and the influence of the rapid localized motion of the $(BH_4)^-$ anion on the conductivity is not known so far, as well as hydrogen transport in general that is crucial for tuning materials' properties for purpose of the energy storage by means of hydrogen.

We investigated the hydrogen dynamics [4] and the electrical conductivity of pure $LiBH_4$ as well as of the $LiBH_4$ based complex hydrides $Li_2(BH_4)(NH_2)$ and $Li_4(BH_4)(NH_2)_3$ in the solid as well as in the liquid state [5]. The two $(NH_2)^-$ containing hydrides show lithium fast-ion conductivities of about 1×10^{-4} S/cm at room temperature. After melting, the total ion conductivities of $Li_2(BH_4)(NH_2)$ and Li4$(BH_4)(NH_2)_3$ increase up to 6×10^{-2} S/cm (378 K) and 2×10^{-1} S/cm (513 K), respectively.

We also investigated the hydrogen release reactions of $LiBH_4$. In the past, different routes were suggested and different intermediate products have been found experimentally. We could show that by carefully choosing parameters such as temperature and applied hydrogen pressure, the preferred decomposition route may be selected [6].

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