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MULTI-FUNCTIONAL ENERGY STORAGE MATERIALS

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Hydrogen is recognized as a potential and extremely interesting energy carrier, which can facilitate efficient utilization of unevenly distributed renewable energy. Furthermore, hydrogen has an extremely interesting chemistry and form compounds with most elements in the periodic table and with a variety of different types of bonds. Metal hydrides has recently become very interesting as new classes of energy materials for batteries and hydrogen storage. Here we report an overview of our recent results within new hydrogen containing materials: (***i***) synthesis of novel metal borohydrides and studies of their properties for hydrogen storage or as ion conductors, (***ii***) tailoring materials properties by anion substitution or neutral molecule derivatives, and (***iii***) *in situ* powder X-ray diffraction studies. We conclude that the chemistry of hydrides is very divers, towards multi-functional materials.

Introduction

We have plenty of renewable energy available but sun and wind are unevenly distributed over time and geographically, therefore energy storage is increasingly important. Metal hydrides have extremely diverse chemistry, structure and reactivity and often high energy density and multi-functionality [1,2].

Results and Discussion

We have recently developed new synthesis strategies and discovered new classes of important 'energy materials', e.g. >30 novel perovskite-type complex metal borohydride, with interesting photophysical, electronic and hydrogen storage properties [3]. Furthermore, anion-mixing provides a link to the known perovskite ABX_3 halides [3]. New metal hydrides, which are fast lithium, sodium and magnesium ion-conductors are also discovered and are now tested in batteries [4,5]. The more stable *closo*-boranes are highly interesting as new solid state ion conductors [6-8]. New synthesis techniques have recently produced series of ammine metal borohydrides, $M(BH_4)_m{\cdot}nNH_3$, *M* = Mg, Ca, Sr, Mn, Y, La, Ce, Gd and Dy, >30 new compounds e.g. the first long series, $Y(BH_4)_3{\cdot}nNH_3$, *n* = 1, 2, 4, 5, 6 and 7 [9-11]. We present new mechanisms for gas release, which depends on the ammonia release temperature and the stability of the metal borohydride. Interestingly, the hydrogen and ammonia content in the released gas appear to have little correlation to the strength of the dihydrogen bonds and the NH_3/BH_4 (*n*/*m*) ratio.

The structures of all new compounds are solved from powder X-ray diffraction, spectroscopy and optimized by DFT calculations and recently reviewed [12]. We demonstrate that structural dynamics in the solid state, i.e. entropy effects, are of extreme importance for detailed material property analysis. We present a 'paddle wheel' mechanism, which may be responsible for fast ionic conductivity [13]. We conclude that the chemistry of hydrides is very divers, towards rational design of multi-functional materials, including new ion-conductors for batteries, hydrogen storage materials, and possibly materials with new types of optical properties.

References

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