



# FLYHY - Fluorine Substituted High Capacity Hydrides for Hydrogen Storage at Low Working Temperatures



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## Targets

At present there is no hydrogen storage system available fulfilling all requirements for use especially in mobile applications:

1. high storage density,
2. temperatures and heats of operation compatible with PEM or HT PEM fuel cells,
3. high hydrogen loading and release rates in the range of a few minutes and
4. low system costs.

FLYHY focuses on these points by

- (i) exploiting findings on tailoring of materials thermodynamics by **anion substitution in alane, borohydrides and Reactive Hydride Composites**, in order to achieve a breakthrough in the thermodynamic hydrogen sorption properties of these materials exhibiting the highest hydrogen capacities known at present,
- (ii) obtaining an **in depth scientific understanding** of the sorption properties of the substituted compounds by extended structural and thermodynamical characterisation and modelling, to optimise the investigated materials,
- (iii) determining tank relevant materials properties like e.g. **compaction behaviour and thermal conductivity of selected compounds**,
- (iv) **scaling-up materials production and doing first tests** in a prototype tank together with a HT PEM fuel cell.

Tailoring of physical properties such as thermodynamics, i.e. working temperatures, and reaction kinetics, is achieved by adding halogens to the storage materials and employing novel paths of materials synthesis.

## Partners

**Helmholtz-Zentrum Geesthacht**  
Centre for Materials and Coastal Research

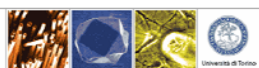


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FLYHY partners at kick-off Meeting, February, 5, 2009, GKSS

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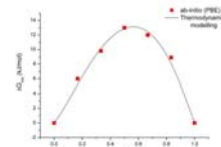
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## Results at end 2<sup>nd</sup> year

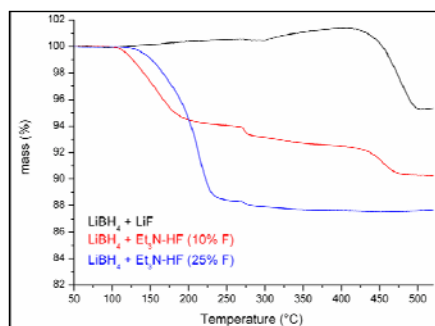
### Fluorine Substitution in AlH<sub>3</sub>

- No F substitution in Alane found
- Reason (theoretical calculations at UNITO see picture to the right): no stable solid solution of AlH<sub>3</sub> and AlF<sub>3</sub>



### Effects of Halogen Substitution in LiBH<sub>4</sub>

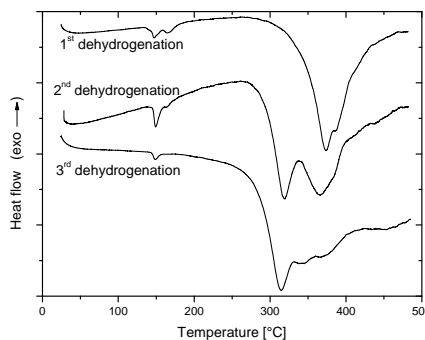
- Cl, Br, and I readily substitute for BH<sub>4</sub><sup>-</sup> groups.
- Mixing of LiBH<sub>4</sub> with F-containing compounds drastically destabilises the borohydride
- No direct substitution of F for H experimentally confirmed so far
- Investigation of sites of F positions, evolving species, and reversibility in progress



Thermogravimetric (TG) curves for pure o-LiBH<sub>4</sub> mixed with LiF and two samples of fluorine substituted LiBH<sub>4</sub> with 10 and 25 % fluorine. A drastic decrease in decomposition temperatures below 150°C is observed, corresponding with fluorine content. Nature of decomposition products so far unknown.

### Effects of F Substitution in Ca-based Reactive Hydride Composite

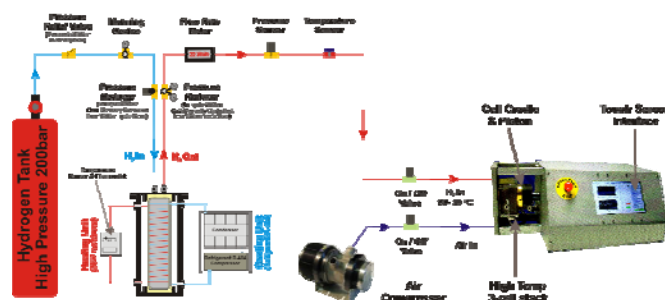
- F addition and cycling lowers start of hydrogen release from above 350°C (pure Ca-based RHC) to below 250°C
- Speed of reaction to be increased
- Investigation of further additives and cyclability in progress



DSC signal of hydrogenated Ca-based RHC, measured at 5 K/min. The onset of hydrogen release decreased over 3 cycles from ca. 300°C to below 250°C.

### Testing of hydrogen storage materials

- Tests of optimised hydrogen storage materials in prototype tank planned in 2<sup>nd</sup> half of 2011 at TROPICAL



## Acknowledgement

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