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Tasks 2.1 and 2.2

New Hydrogen Storage Materials Development

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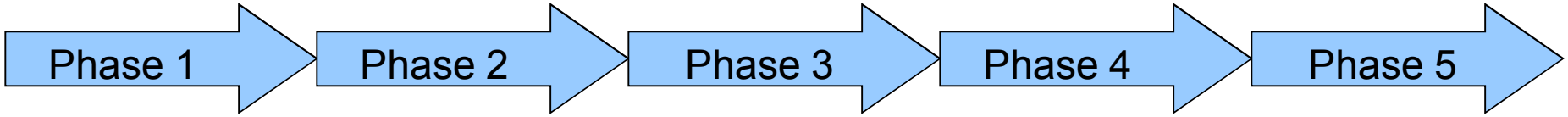
Strategy for discovering new practical metal hydrides



Screening	Na-Si-H	$Ca(BH_4)_2$	K_2LiAlH_6
On-going	*6-9wt%*	*11wt%*	*5wt%*

Phase 1: *Discover new metal hydrides by screening at the high-pressure station*

Phase 2: *Optimize synthesis route and structural characterization*

Phase 3: *Investigate hydrogen storage properties; H-content, sorption temperature*

Phase 4: *PCT-measurements; thermodynamics and kinetics*

Phase 5: *If needed the material may have to be further modified to improve H-sorption properties*

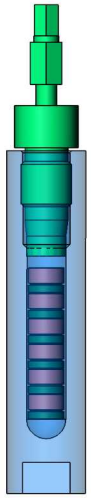
Synthesis@High-pressure station

Solid state synthesis at High-pressure station: <20,000psig, <500°C

This method is the most efficient way to discover new complex type metal hydrides

Sample preparation

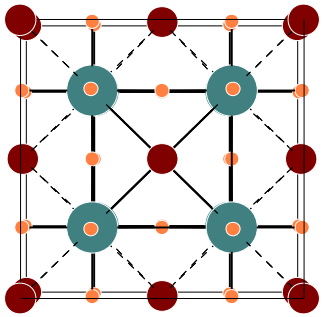
- High-energy ball milling
- Press pellets to place in the steel crucibles
- Heat treatment under High H_2-pressures



Reactor vessel with 6 steel crucibles

Characterization

XRD reveals New material's structure



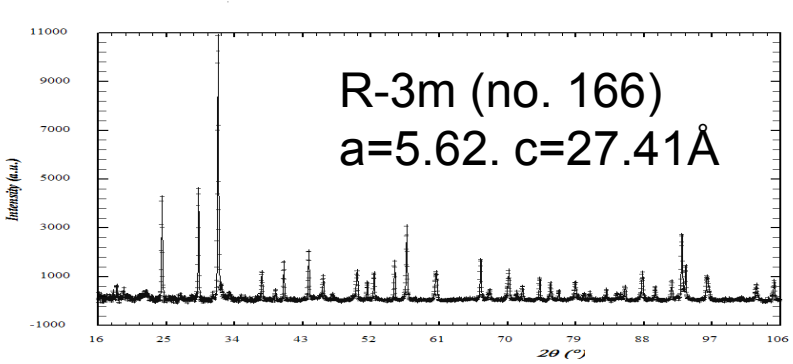
Discovered New Materials during the 1st year

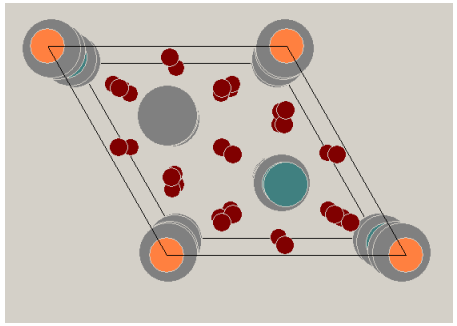
1. Bialkali Alanate K_2LiAlH_6 5wt%
2. Calcium Borohydride $Ca(BH_4)_2$ 11wt%
3. Ternary Si-system 6-9wt%

A New Bialkali Alanate K_2LiAlH_6

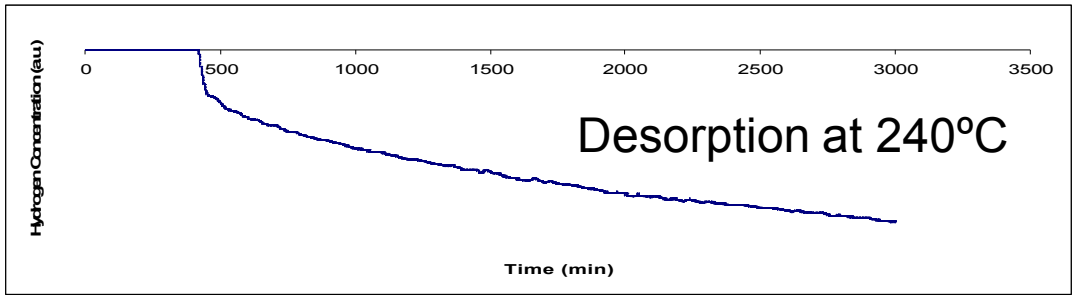
A new bialkali alanate was synthesized by heating under H_2-pressures

With Rietveld refinement the structure was shown to be isostructural with HT-K_2LiAlF_6





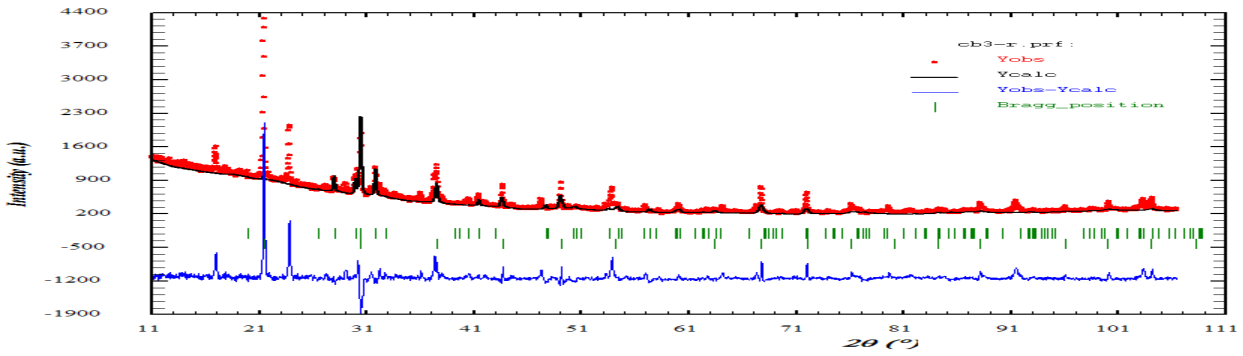
K: grey
Li: orange
Al: green
H: red



Maximum H_2-capacity is 5.1wt%, but
$K_2LiAlH_6 \rightarrow 2KH + LiH + Al + 2H_2$ results in reversible 2.6wt%

Calcium Borohydride

- $Ca(BH_4)_2$ contains 11.5wt% hydrogen!
- *Potential stable structure was predicted by theoretical modeling!*
- Made in the solid state at high H_2-pressures:
  $CaB_6+2CaH_2+10H_2 \leftrightarrow 3Ca(BH_4)_2$
- Reproduction and structural characterization is on-going.
- Hydrogen sorption experiments show partial reversibility: Desorption at 240C, absorption at 390C.
- Next step: Modify the compound to facilitate reversibility.



Ternary Silicon Hydrides

- No complex type ternary Si-hydrides are known!
- Potential for 6-12wt% hydrogen
- Potential anionic complex: $[SiH_6]^{2-}$ may be stabilized to form Li_2SiH_6, Na_2SiH_6 or $CaSiH_6$. Or perhaps $LiNaSiH_6$, $LiKSiH_6$ etc.
- Other potential symmetries of Si?
  - Ex: $[Si(4)H_5]^-$, $[Si(3)H_4]^-$, $[Si(2)H_4]^{2-}$, $[Si(2)H_3]^-$.

- New phase appeared in the Na-Si-H system!
- Finding a better synthesis route to increase the yield is on-going.
- Next step: characterization to understand if the new material is useful as a hydrogen storage material.

K_2LiAlH_6 as a role model for predicting stable metal hydrides

- *We need new methods to predict which metal hydride systems that are likely to show new materials.*
- *K_2LiAlH_6 was chosen as a role model since it was recently synthesized and structurally characterized at Sandia.*
- *The structure of K_2LiAlH_6 was determined from experimental data and it was shown to have the lowest minimized energy by a Monte Carlo method.*
- *We will now continue screening for new metal hydrides at the high-pressure station and test hydrogen sorption properties and use theoretical modeling as a guidance to select stable, light-weight, high-capacity metal hydrides. Further details will be presented by Eric Majzoub.*