BOR4STORE
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http://www.bor4store.eu

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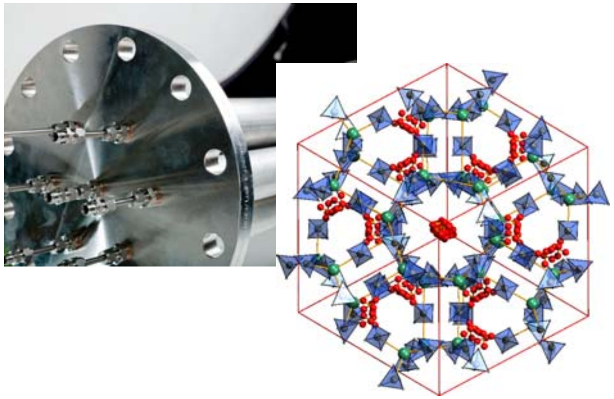
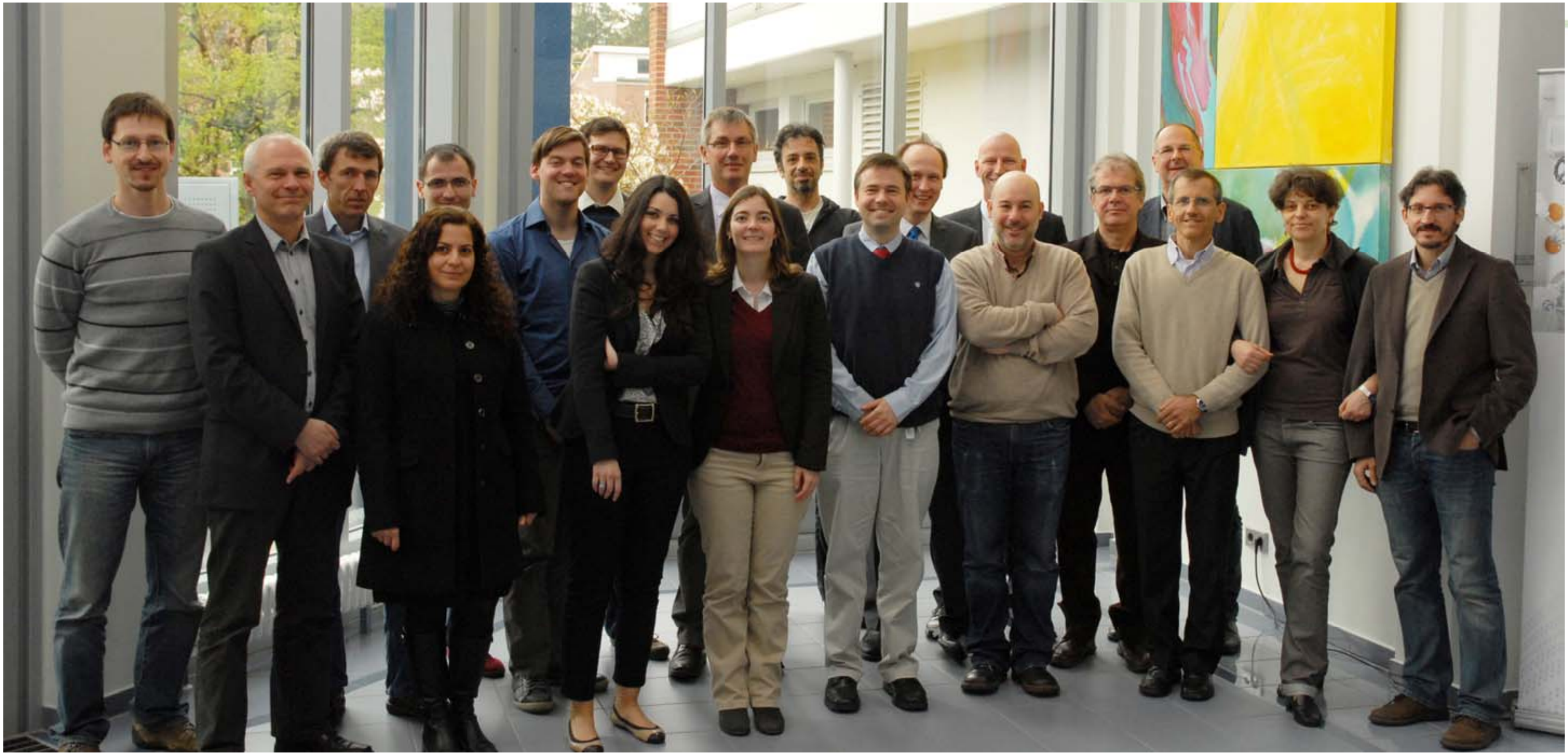


General Overview

– full title: **“Fast, reliable and cost effective Boron hydride based high capacity solid state storage materials”**
– runtime: **April, 1st, 2012 – March, 31st, 2015**
– total budget **4.07 Mio.€**
– FCH JU contribution **2.274 Mio.€**

– **3 industry partners** (2 SME, 1 Non-SME, latter NEW-IG member)
  - SME: Zoz GmbH (GE), Katchem spol. s.r.o. (CR)
  - Non SME Abengoa Hidrógeno (ES)
– **6 research Institutes** (3 N.ERGHY members)
  - Helmholtz-Zentrum Geesthacht (DE), Aarhus Universitet (DK), Institutt for Energieteknikk (NO), Unversità di Torino (I), Empa (CH), National Centre for Scientific Research “Demokritos” (GR)
– **www.bor4store.eu**

The people



Project goals and targets

- a novel solid state hydrogen storage prototype system based on **boron hydrides**
  - system capacity **> 40 kg H_2/m^3 , > 4 wt.%** with priority on volumetric capacity
  - suitable for typical load cycles of **SOFC in net independent power supply**
  - cycling stability >98% of capacity over at least 500 loading-unloading cycles
- **cost effective production route** of the best hydrogen storage material
  - use of low purity raw materials, **cost effective materials** processing
  - demonstration of potential for **system cost of 500 €/kg** of stored H_2
- **Bi-annual materials downselection** decision, based on
  - **materials performance** key indicators and **cost perspectives**
- setup of a **laboratory prototype**
  0.1 - 1 kW SOFC integrated with a 100 - 1000 Nl hydrogen storage system
  - model for a **continuous power supply** for net independent applications
  - **techno-economcal evaluation** compared to compressed gas storage and other fuel cell technologies, respectively:
    - improved storage capacity and overall energy efficiency
    - decreased total cost of ownership
- an indicator of **allowable hydrogen purity** for stable storage properties
- demonstrating techno-economical **readiness of solid state hydrogen storage**

Approach in performing the activities

- synthesise **novel boron hydride based materials** (capacities >8 wt.% and >80 kg H_2/m^3)
  - Bi- and tri-metal cation substituted boron hydrides
  - Anion substituted boron hydrides
  - Composites (e.g. Eutectically Melting and Reactive Hydride Composites),
- accelerate **reaction kinetics** and adjust **reaction temperatures**
  - supply an SOFC with sufficient hydrogen pressure and flow at acceptable rehydrogenation times of 1 hour or below
  - investigate effects of additives on rate limiting reaction steps
- enhance the **cycling stability** of the materials to several **1000 cycles**
  - suitable additives
  - scaffolding the storage material in pore size optimised porous materials to tailor reaction pathways, prevent phase separation and retain a high storage density,
- decrease **materials cost** (potential for **< 50 €/kg** in large scale production)
  - develope cost effective materials synthesis routes
  - investigate effects of impurities on storage properties
    $\Rightarrow$ enable use of cost effective raw materials
- construction of a boron hydride based **laboratory prototype tank** ca. 100 – 1000 g of storage material, **supply** a 0.1 - 1 kW **SOFC**
  - demonstrate stability of system performance over 500 load cycles

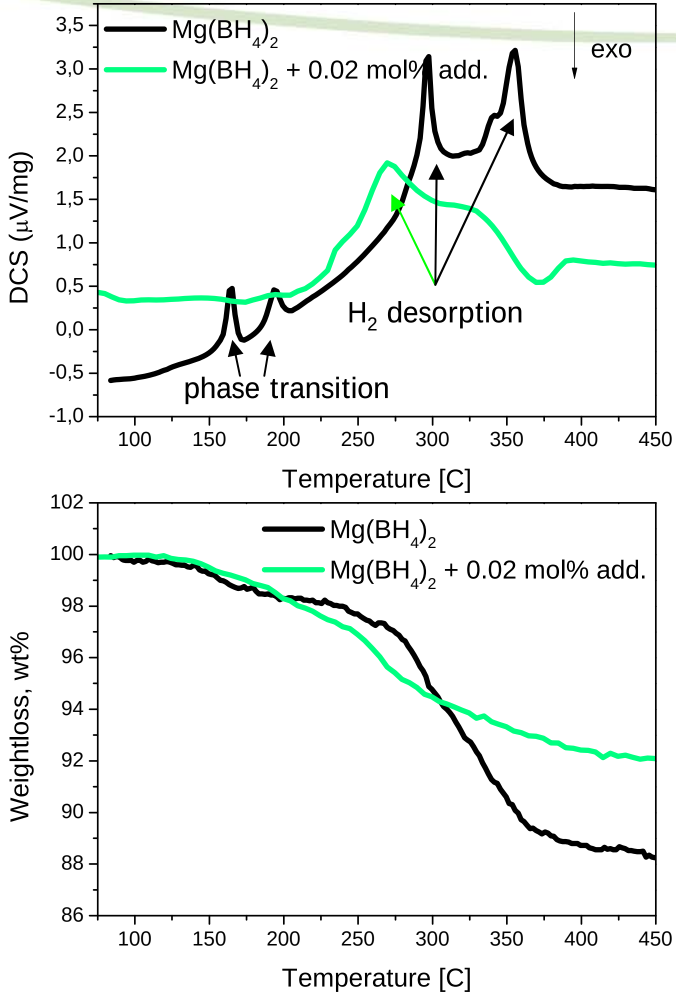
Testing Procedures

- in-house test procedures or non-standardized test procedures
  - materials **capacities** and reaction **kinetics**:
    - hydrogen uptake and release (mostly Sievert’s type machines)
    - Differential Scanning Calometry
    - Temperature Programmed Desorption
    - Thermogravimetric Analysis
  - materials **microstructures**
    - *ex and in situ* powder X-ray and neutron diffraction
    - *ex and in situ* Raman spectroscopy
    - *ex and in situ* Infrared spectroscopy
    - nuclear magnetic resonance, electronic paramagnetic resonance
  - **thermal capacity** and **conductivity**
  - release of **volatile species** by *in situ* mass and infrared spectroscopy
  - **Hydrogen Tank Test Facility** at HZG
  - Test facility for **integrated SOFC – hydrogen tank system** at Abengoa Hidrógeno
- standardised test procedure
  - **certified tank construction** according to national and international standards on pressurised containers $\Rightarrow$ testing of tank hull

γ-$Mg(BH_4)_2$: study of additives

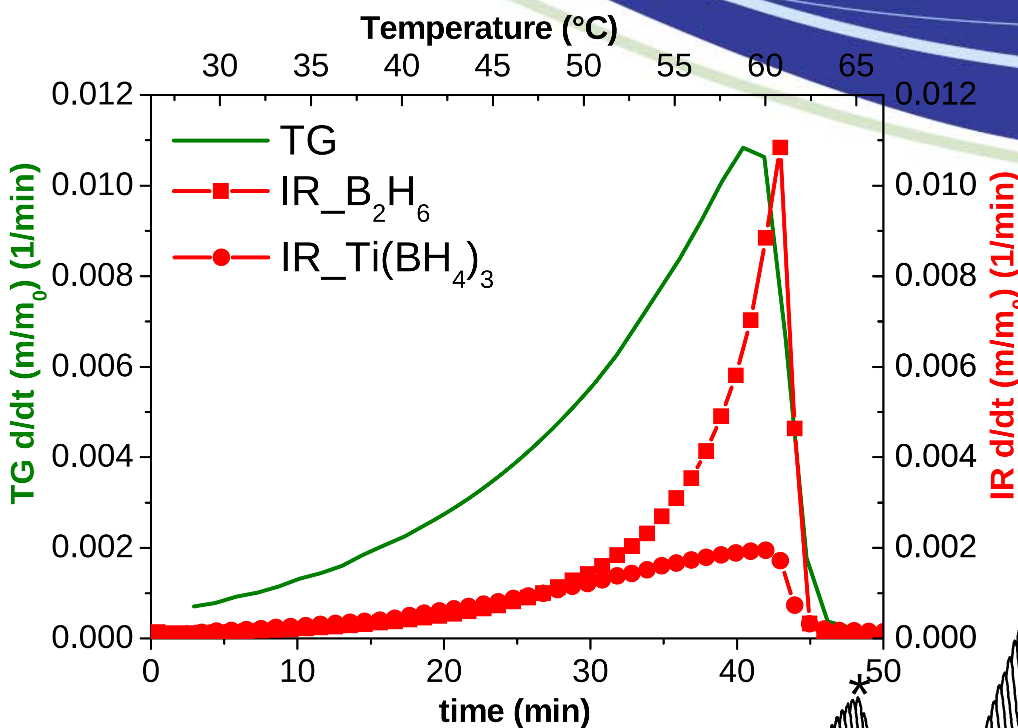
IFE, WP1, WP2, deliverable D4.1

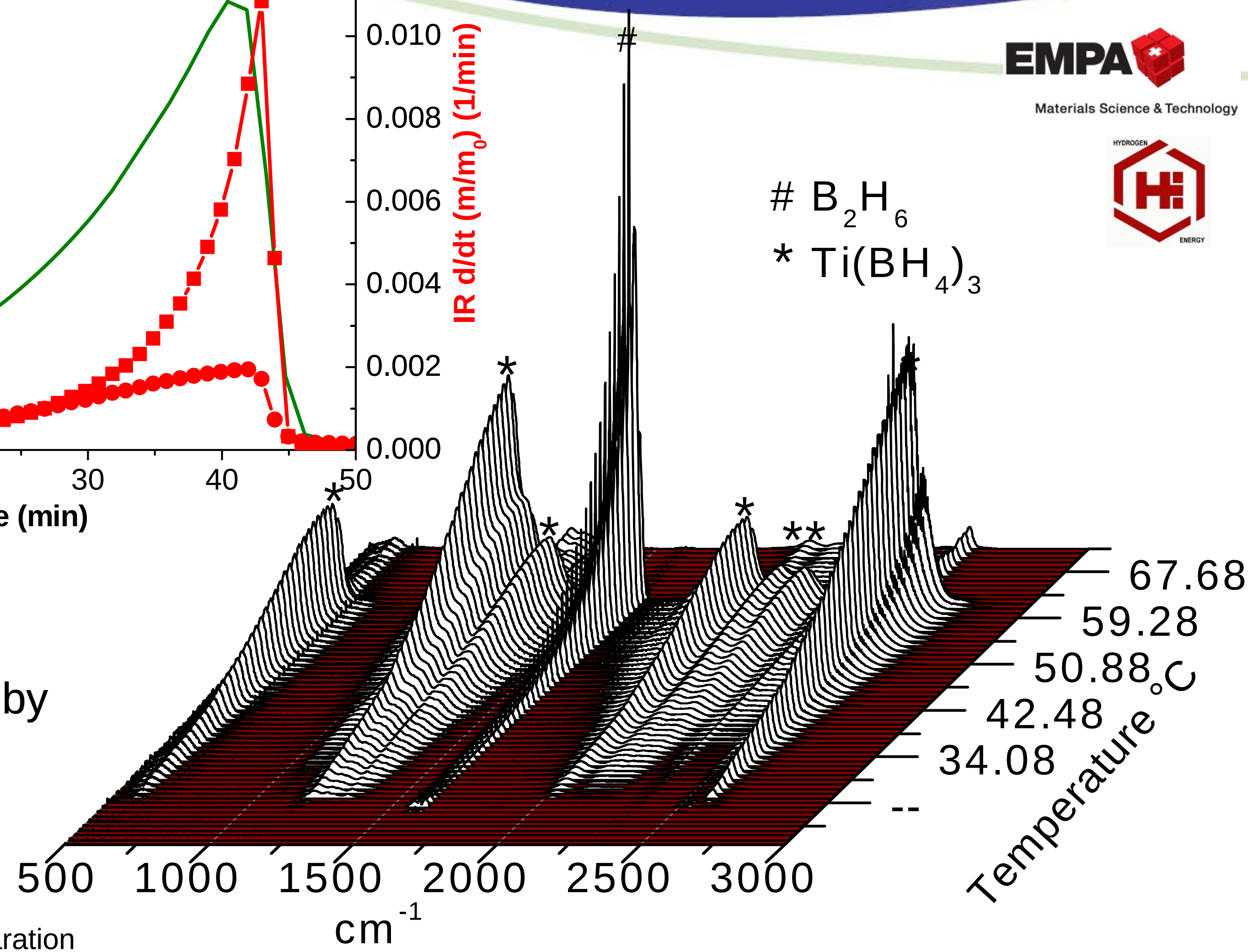
- Effect of additives in decomposition of $Mg(BH_4)_2$
  - NbF_5 additive
    - H_2 release temperature decreased (ca. 30°C)
    - different desorption scheme
      - no phase transition below 200°C
      - just one broad desorption peak
    - rather high gravimetric H_2 content of 8 wt.%
  - reasons for this behaviour under investigation
    - *ex and in situ* X-ray diffraction



Decomposition of $Ti(BH_4)_3$

Empa, WP2





In situ IR

$Ti(BH_4)_3$ decomposes by release of diborane

E. Callini, et al., manuscript in preparation

ab initio calculations $Mg(BH_4)_2$

UNITO, WP3

First results on the study of phase stability

- Comparison among **six** different phases: experimental (α, γ and δ) and theoretically predicted ones
- In agreement with experiment and previous calculations [1], the most stable phase is the **α-phase** (correct order of stability: α > γ > δ)

Next steps:

- **Surface stability of different faces of the α-phase**

Slab models from 3D structure

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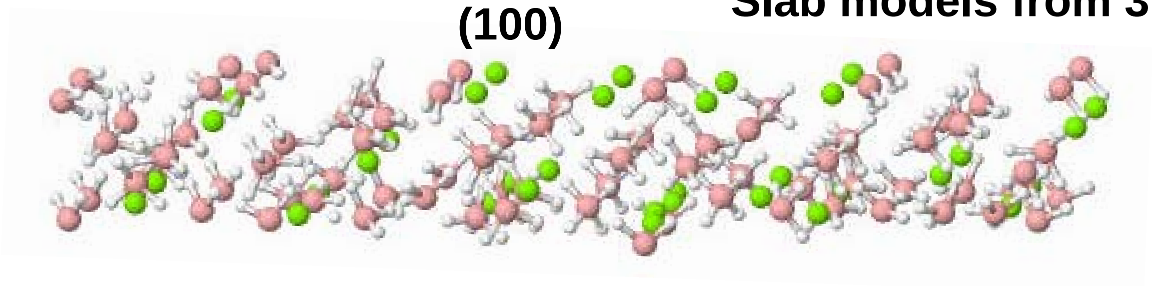

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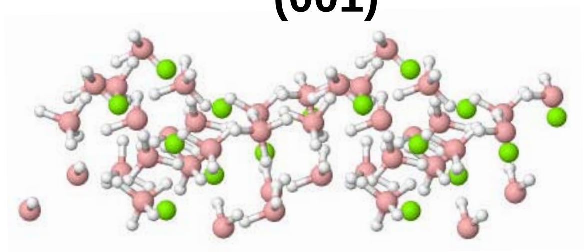
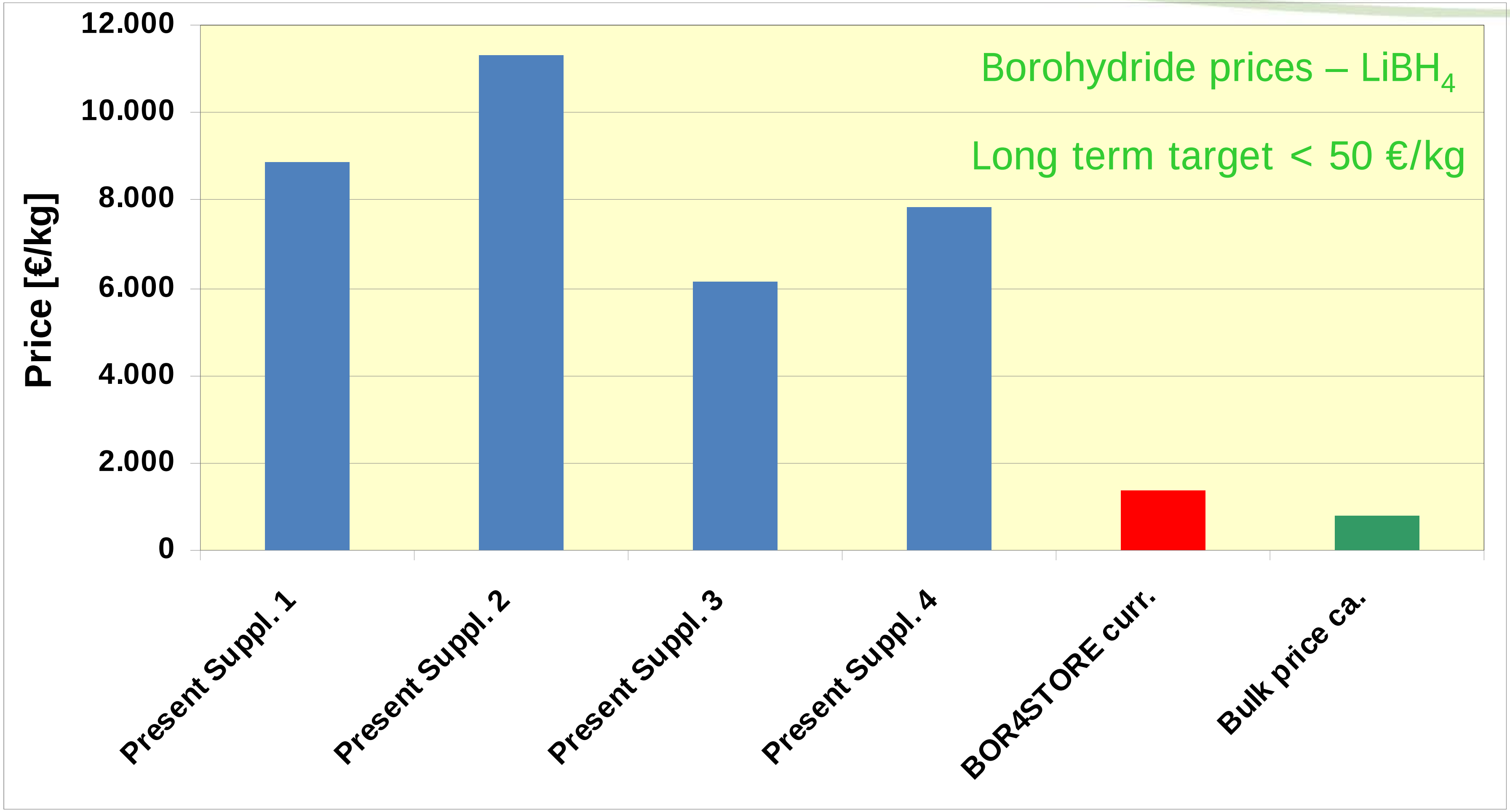


- **Role of the additives (e.g. TM):**
  - in the bulk (supercells with point defects)
  - at the surface (slab models with point defects)

[1] A. Bil, B. Kolb, R. Atkinson, D. G. Pettifor, T. Thonhauser and A. N. Kolmogorov, Phys. Rev., B 83, 224103 (2011)

Materials cost

Katchem, Zoz, WP4

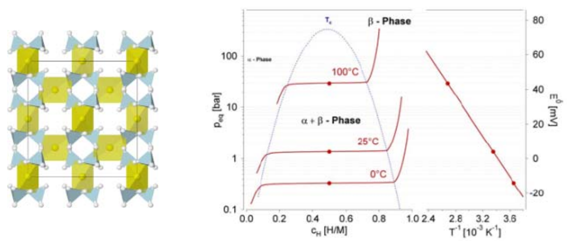


Techno-economical evaluation of a combined SOFC – solid state hydrogen storage system

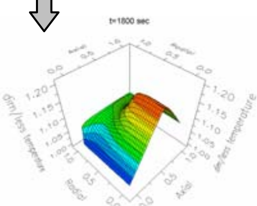
☛ **Development of a simulation model of the whole system including a thermo-chemical model of the storage material**

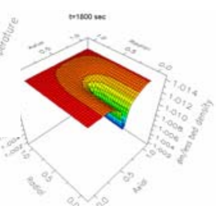
Simulation of stand-alone MHT system

Material properties



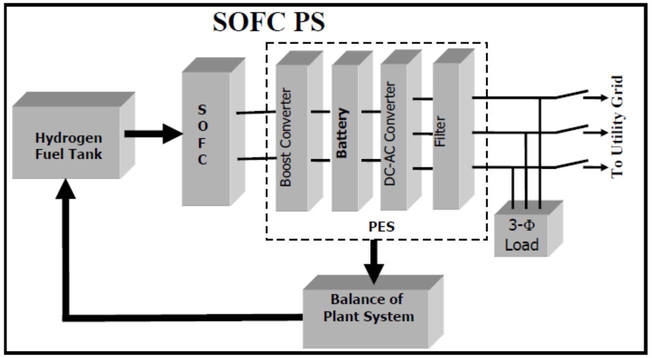
Optimised tank design

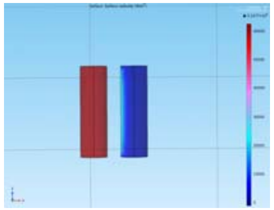




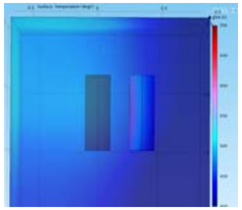
temperature & density temporal profiles in the MH bed

Coupling of SOFC- MHT systems





Radiative heat flux on the MHT



Temperature profile of radiating SOFC

dynamic process simulation and optimization software: gPROMS, COMSOL

Prototype tank construction

HZG, WP5

- 1^{st} generation prototype tank: $LiBH_4$ – MgH_2 Reactive Hydride Composite
  - Designed, constructed and built at HZG
  - Ca. 250 g of storage material
    ⇒ ca. 22 g / 250 Nl H_2
  - External heating by heating jacket (front) or oil bath (back) possible
  - Temperature of operation ca. 350°C with heating jacket
  - Loading time app. 1 h at 50 bar of hydrogen
  - 2^{nd} generation tank constructed and under testing (ca. 500 g of material)

Correlation of the project with AA2 (MAIP/AIP)

From original text of MAIP:

- long-term and breakthrough orientated research on
  - improved hydrogen storage based on
    solid materials for increased energy efficiency and storage capability.
- Some of these technologies are ready for implementation in small and medium scale stationary applications,
  - e.g. in combination with high temperature fuel cells.
- Here, the main development targets will be
  - energy efficient integration and a
  - significant reduction of cost of the storage systems
- involvement of SMEs in its activities
  - Zoz, Germany
  - Katchem, Czech Republic

Project activities vs. MAIP/AIP

- Cost reduction
  - MAIP Page 7: Targets for storage of hydrogen in solid materials:
    - 2010: 3 t cap. | 5 M€/t, 2015: 5 t cap. | 1.5 M€/t , 2020: 10 t cap. | 0.85 M€/t
  - At present:
    - RT hydrides: ca. 3.500 €/kg of stored hydrogen
    - Boron hydrides: ca. 5.000 - 10.000 €/kg possible with certain compounds
    - Reason
      - today: high purity raw materials, kg scale production (>> 1000 €/kg)
      - tomorrow: less pure raw materials & ton scale production (<< 100 €/kg)
- FCH JU Call 2011, Topic 2.4
  - Hydrogen storage for supply of SOFC systems for stationary (e.g. net independent power supply, CHP)
  - break-through basic research on hydrogen storage materials
  - development of storage systems
  - improvement of storage capacity etc.
  - cost reduction by use of less pure raw materials and improved cost efficient methods of synthesis

Gaps/Bottlenecks in RTD&D

- Cross-Cutting issues
  - Integration of Hydrogen Production from Renewables / Hydrogen Storage / Hydrogen use (FC, ICE, direct hydrogen use e.g. in glassworks etc.)
- PNR/RCS
  - Extension of ISO 16111 “Transportable gas storage devices – Hydrogen absorbed in reversible metal hydrides” to
    - high capacity materials, also for stationary applications
    - higher temperatures of operation (ca. 300 – 400 °C)
    - higher pressures (100 - 150 bar)
- Priorities and topics possibly under/over-estimated in the AIPs in terms of technical challenge
  - Underestimated
    - AA2 “Hydrogen production and storage” as a whole has too low budget
    - low pressure, large volume hydrogen storage beyond the 5 – 10 kg scale
    - total energy efficiency of the chain from hydrogen production over storage to use
  - Overestimated
    - need for demonstration projects - take too much of the FCH JU budget

Contribution to Cross-cutting issues

- Training and Education:
  - 6 PostDoc or PhD positions
  - Public Final Dissemination Seminar and Workshop
- Safety, Regulations, Codes and Standards
  - Agreement on harmonized materials testing procedures
  - Complete System Design according to international rules for pressurized containers and systems
- Dissemination & public awareness
  - www.bor4store.eu
  - Press release upon project start
  - Presentation at N.ERGHY GA, May 2012, Prague
  - Presentation at Int. Conferences (e.g. MH2012, Japan)
  - Joint SSH2S, BOR4STORE, EDEN & HYPER projects workshop planned for 2013/2014
  - Presentation at Int. Trade Fairs planned (FC Expo 2013 (JP), Hanover Fair 2013 (DE)), FCH JU SA 2013, …
  - Public Final Dissemination Workshop, 2015
- Information on publications; information on patents
  - N.a. yet due to short runtime

Technology Transfer / Collaborations

- **Technology transfer**
  - Results of project to be **commercialised by industrial partners** and/or joint ventures
    - materials processing: Zoz, Katchem
    - materials production: Katchem, Zoz
    - hydrogen storage tanks: Zoz
    - hydrogen based net independent power supplies: Abengoa Hidrógeno
- **Collaborations**
  - **Joint SSH2S, BOR4STORE, EDEN & HYPER projects workshop** planned for 2013/2014
  - BOR4STORE partners member of **H2FC infrastructure project** (IFE, NCSRD, EMPA) and **COST Action MP1103** "Nanostructured materials for solid-state hydrogen storage" (HZG, AU, IFE, EMPA, NCSRD)
  - BOR4STORE partners member or **coordinator of national projects** (e.g. HyFillFast (DK), ATR (DE), …)
  - Several partners members of **local and national organisations (e.g. EERA JP "Energy Storage", SP "Chemical Storage", or IEA HIA Task 22)**

Project Future Perspectives

- Future research approach and relevance
  - Cost decrease by novel production routes
  - Scale-up and setup of net independent power supply demonstrator
  - Integration of Integrated MH-Tank–SOFC into other stationary and quasi-mobile applications (trains, ships, …) with medium scale storage of hydrogen (>> 10 kg)
- Need/opportunities for increasing cooperation at EU, Member States or Regional level, and/or for building alliances between industry, government, research centers, SMEs, etc.
  - Transfer of project results to
    - Industrial exploitation
    - Adaption to other applications
    - demonstration
- Need/opportunities for international collaboration
  - Collaboration with US, Japan, Korea, ICPC countries, on cost effective hydrogen storage technologies
- Possible contribution to the future FCH JU Programme
  - Technologies for cost effective storage of hydrogen to reach or outperform the 2015 and 2020 targets for hydrogen storage in solid state materials based tanks