NANOHy
(Grant # 210092)

Novel Nanocomposites For Hydrogen Storage Applications

7th FP

Maximilian Fichtner
Karlsruhe Institute of Technology (KIT)
m.fichtner@kit.edu

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Novel Nano Composites for Hydrogen Storage Applications

Consortium

	Beneficiary name	Beneficiary short name	Country
1	Karlsruhe Institute of Technology	KIT	Germany
2	CNR-ISC Firenze	CNR	Italy
3	CNRS	CNRS	France
4	FutureCarbon GmbH	FC	Germany
5	Institutt for Energiteknikk	IFE	Norway
6	Max-Planck-Institut	MPI-KGF	Germany
7	NCSR Demokritos	NCSRD	Greece
8	University of Oslo	UniO	Norway
9	Korean Institute of Science and Technology	KIST	South Korea

Beginning	Duration	End	Budget (M€)	Partners
Jan 1, 2008	48 months	Dec 31, 2011	3.1 Total 2.4 EC contrib	8 research 1 industry

Motivation

- Practical problems due to the limitations of the current storage systems (although high theoretical capacity exists).
- Lack of understanding of the properties of hydrides on the nanoscale.

Three major problems of H storage materials are adressed in NANOHy:

- Improvement of kinetics of the H exchange (lower working T, p)
- Tuning of thermodynamics (equilibrium properties)
- Safety (e.g. stable in air)

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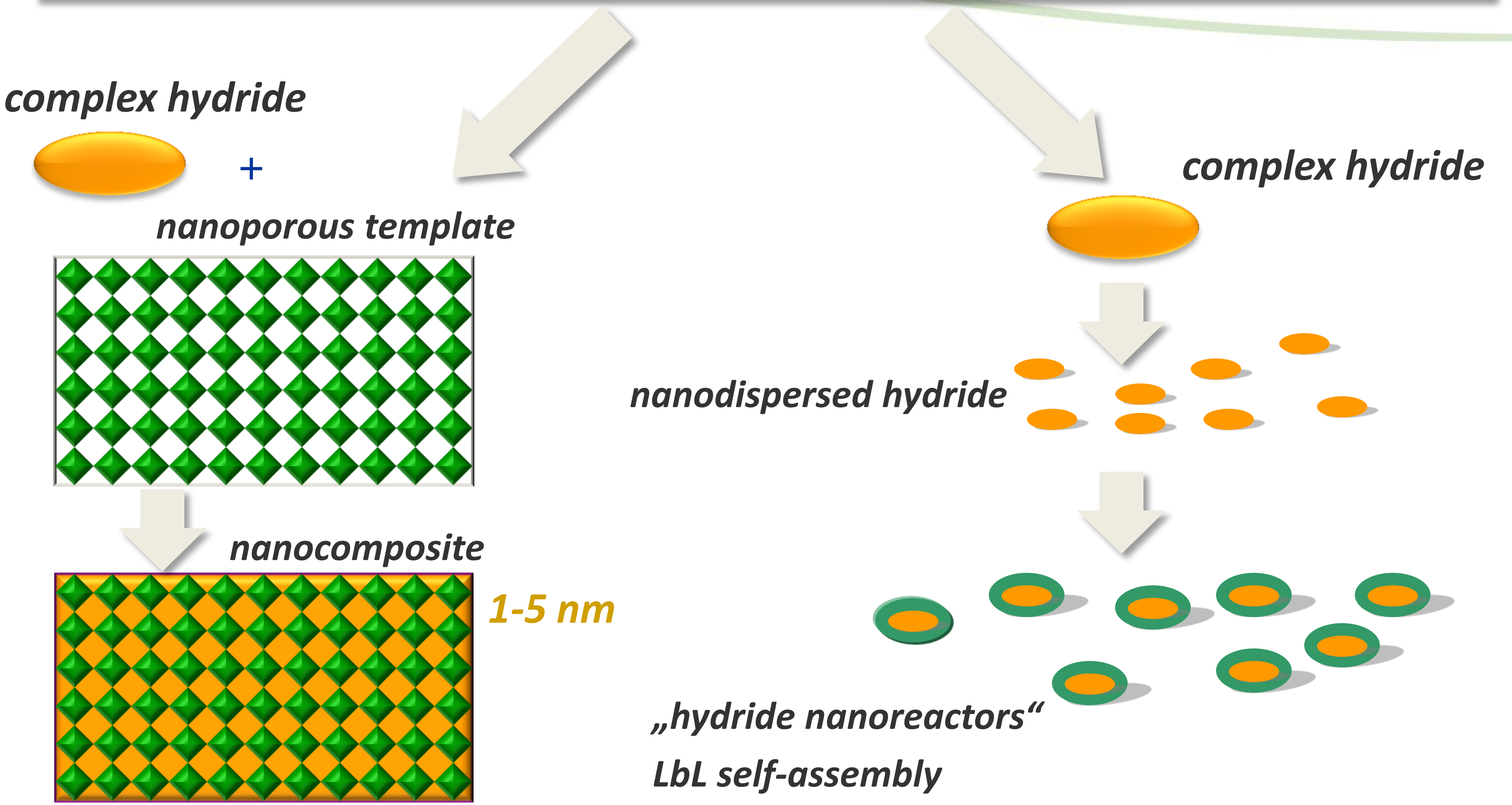
Targets

Parameter	Unit	Target
Particle size of nanodispersed complex hydrides	nm	< 5
Gravimetric density (ref. to materials weight) at 100-200°C	mass% H	> 8
Refuelling rate	g/s	0.5
Desorption temperature of H_2	K	Lowered by > 50 K compared to ball-milled material; targeted temperatures are < 200 °C
Reaction enthalpy ($\Delta H_{reaction}$)	kJ/mol H_2	30-40
Amount of material produced	kg	Batches of 0.5 kg - 1 kg in WP 5.
Reduction of desorbed diborane	%	> 90
Safety	-	No self-ignition in contact with air.
Tank	-	At least 1 laboratory test tank for 0.5-1 kg of material

Strategy and Approach

Make use of size effects and encapsulate the hydrides at the lower nanoscale



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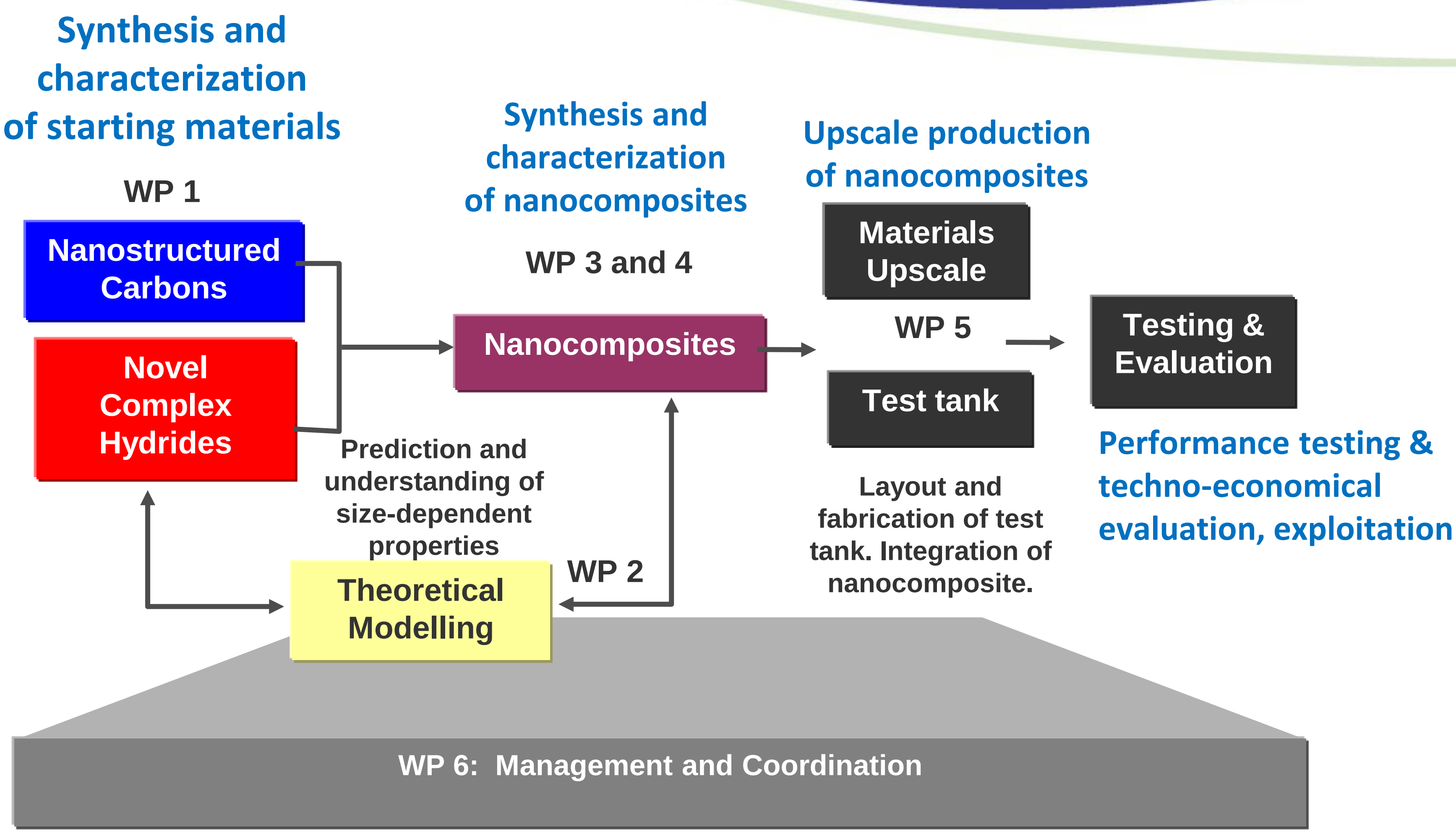
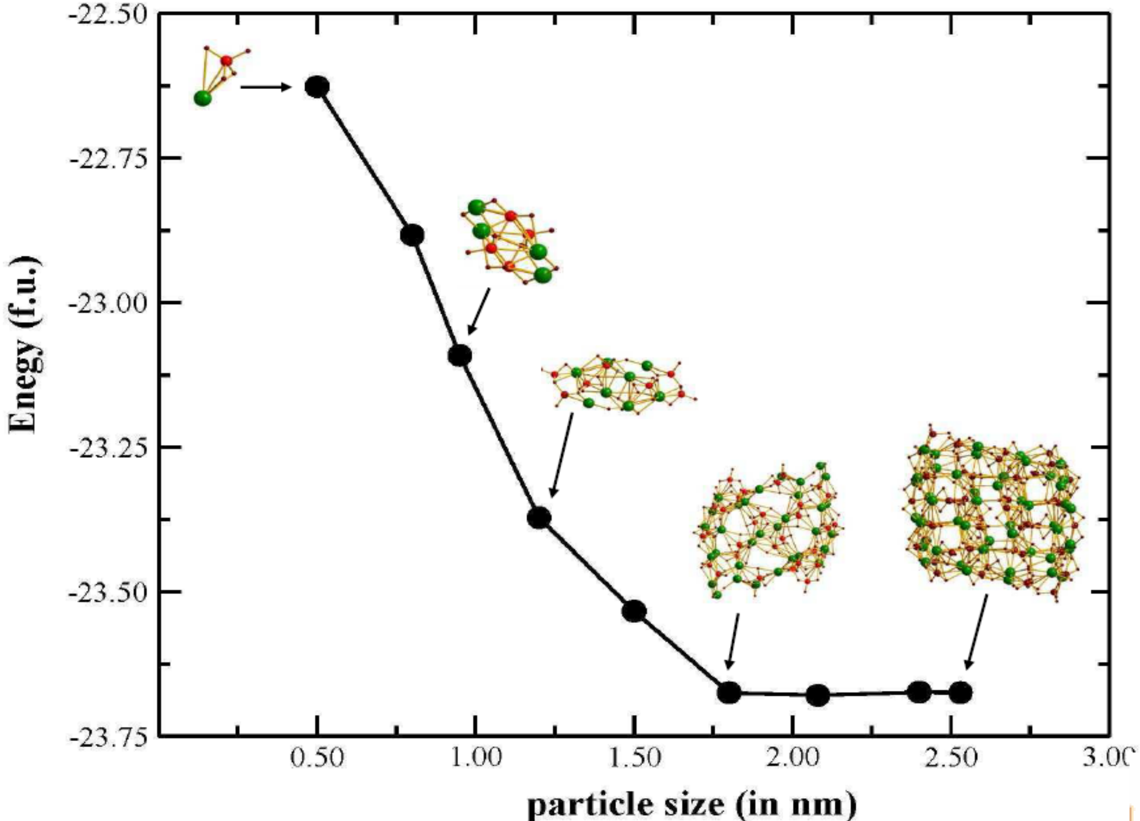
Project Plan



Results

Modelling / Critical particle size of nanoclusters



nano-clusters

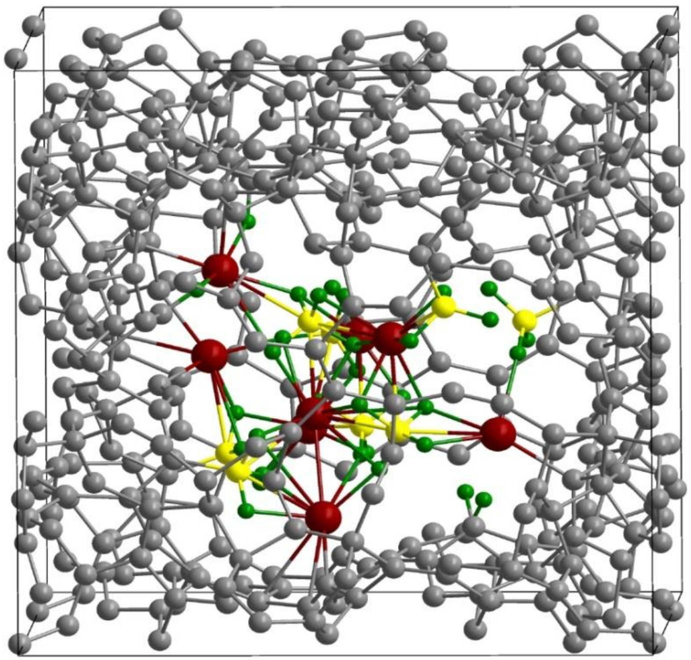
critical size

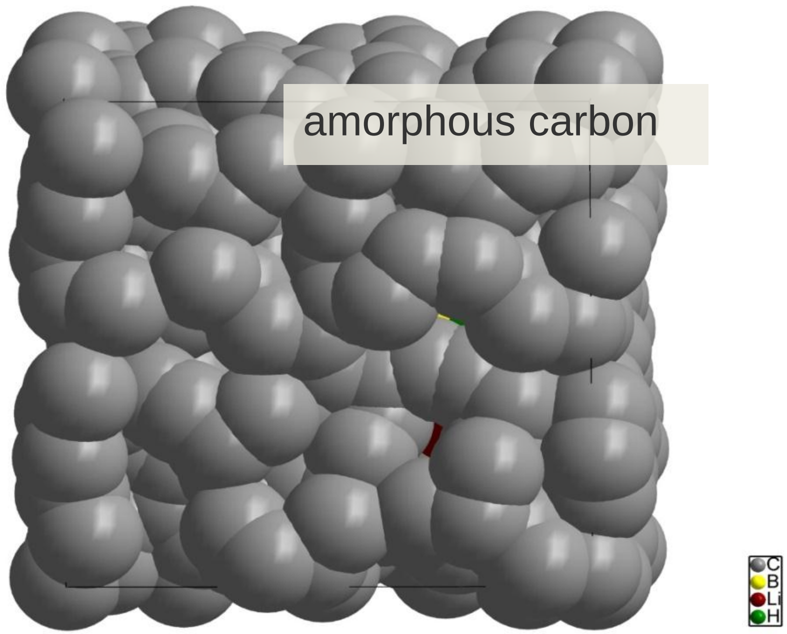
$LiBH_4$	1.75 nm
$NaBH_4$	1.35 nm
KBH_4	1.80 nm

SMN SENTER FOR MATERIALVITENSKAP OG NANOTEKNOLOGI

Results

Modelling / $LiBH_4$ in 2 nm C pore





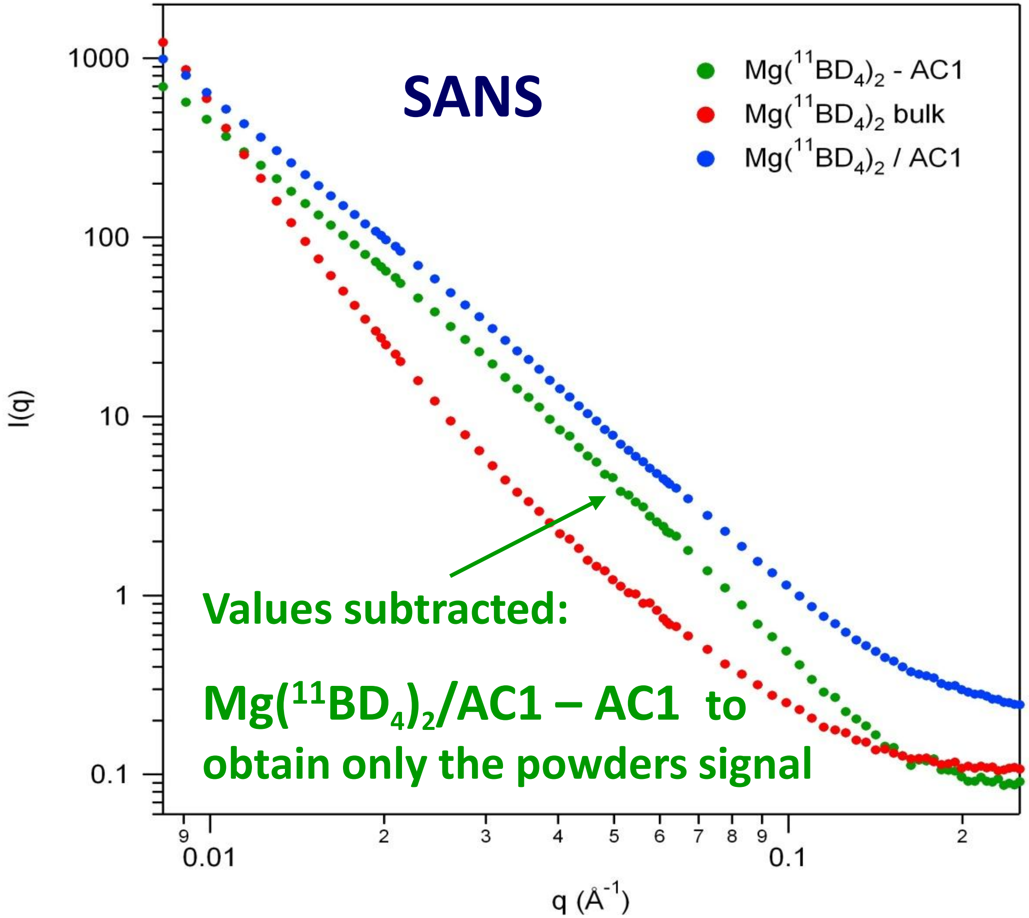
Structure of the material in the void is entirely different from bulk structure and from structure of particle in vacuum → new effects !

First published by:

Vajeeston *et al.*, Nanotechnology (2009)

Results

IFE   KIT Karlsruhe Institute of Technology



Small Angle Neutron Scattering

$Mg(^{11}BD_4)_2$/activated carbon

$Mg(^{11}BD_4)_2$ bulk powders

Subtracted intensities $Mg(^{11}BD_4)_2$

First direct proof of succesful infiltration of complex hydrides in < 2nm pores !

Sartori *et al.* Nanotechnology (2009)

Sartori *et al.* J. Phys. Chem. (2010)

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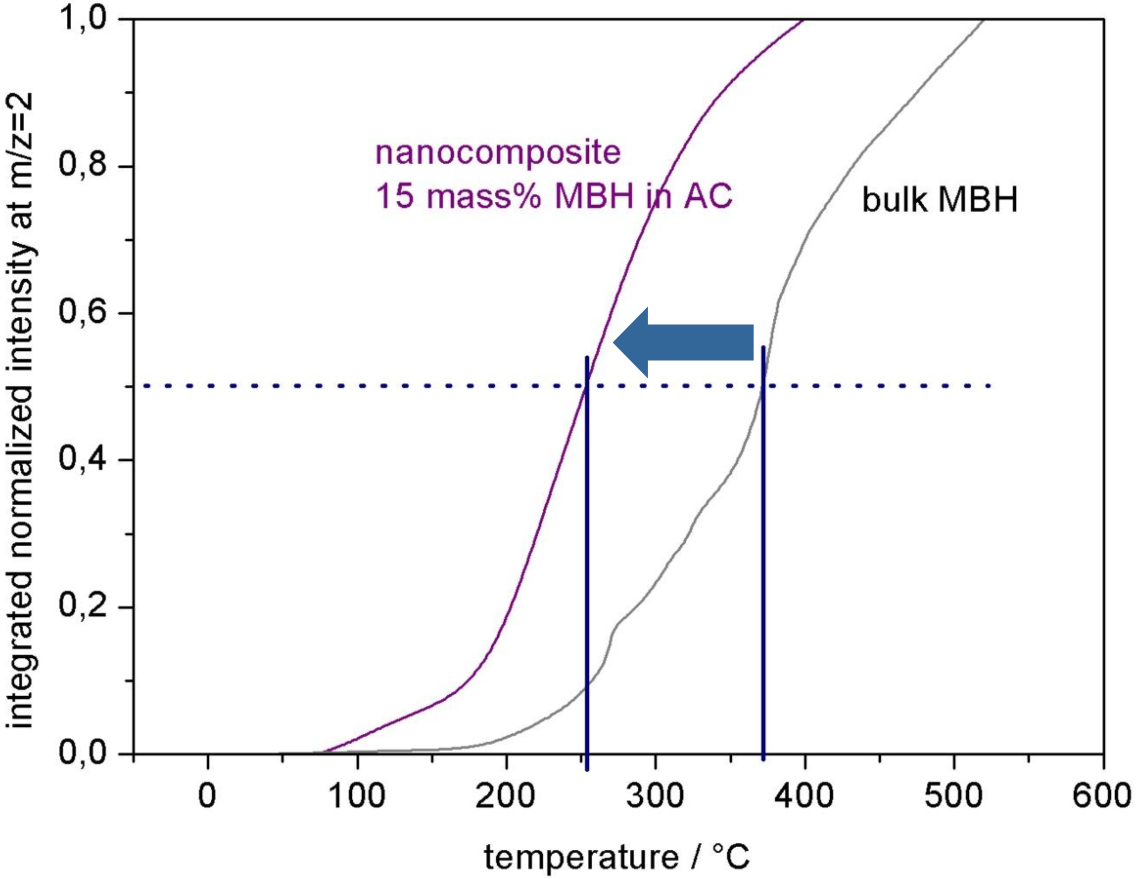
Results

Improved Kinetics



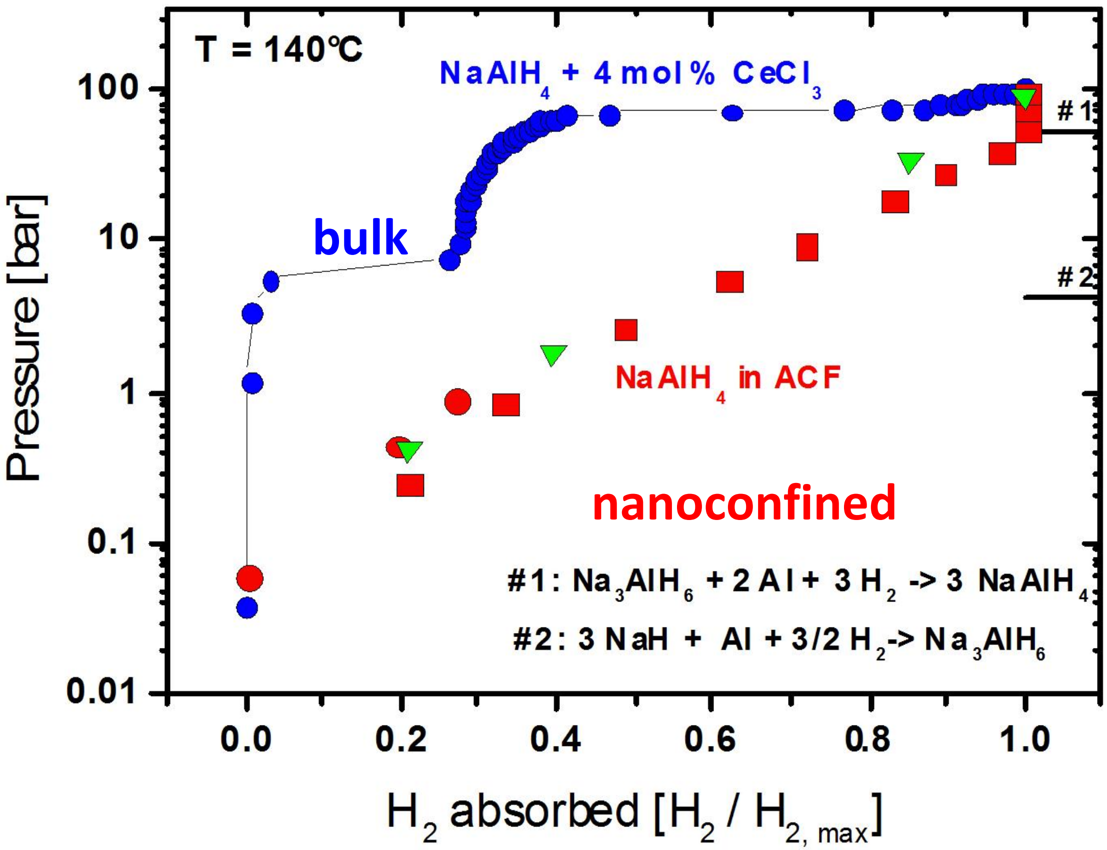
T shift of the H desorption by 120 K to lower temperatures !

Karlsruhe Institute of Technology

Fichtner *et al.* Nanotechnology (2009)

Results

Altered Thermodynamics 1



First experimental proof for modification of thermodynamics and reaction pathway of a nanoconfined complex hydride.

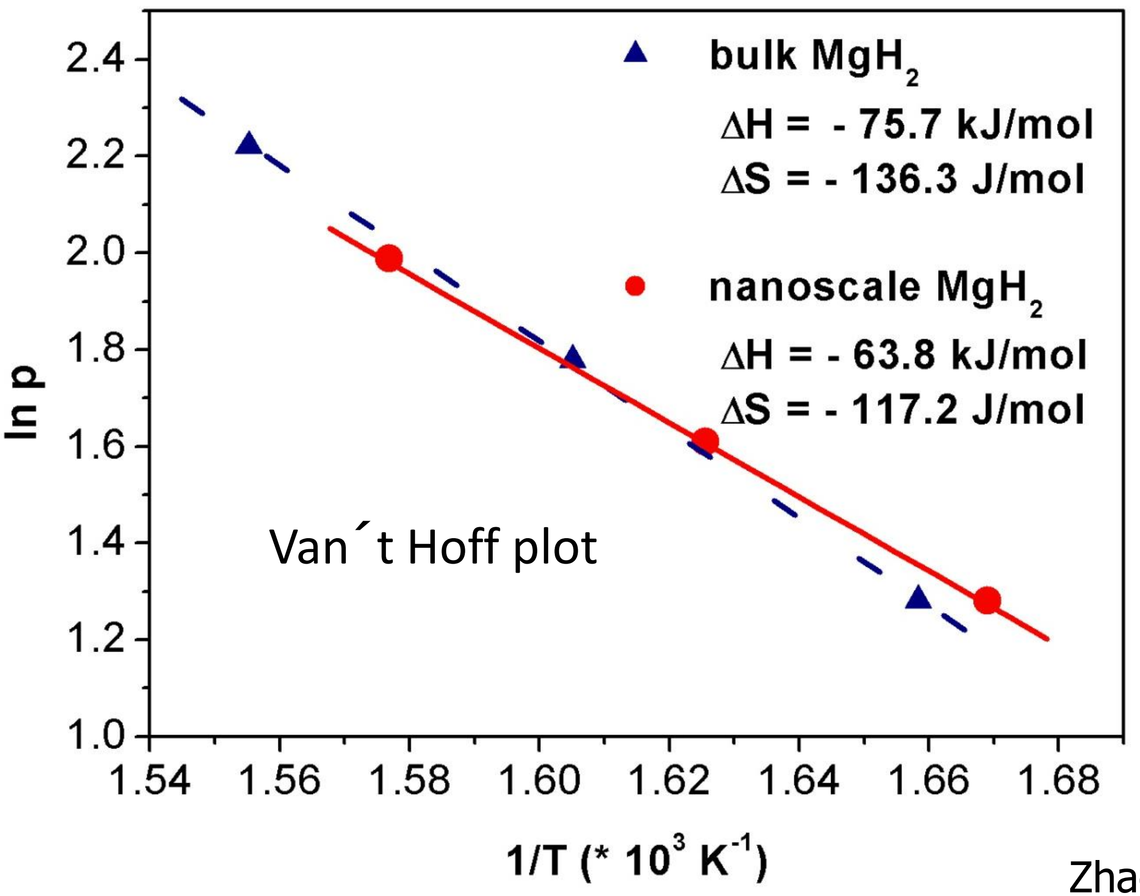
→ Fits to predictions of our modeling group.

Fichtner *et al.*, MH (2008)

Lohstroh *et al.* ChemPhysChem (2010)

Results

Altered Thermodynamics 2



Changes:

ΔH lowered by 11 kJ/mol

ΔS lowered by 19 J/mol

First experimental proof for alteration of thermodynamics of nanoconfined MgH_2.

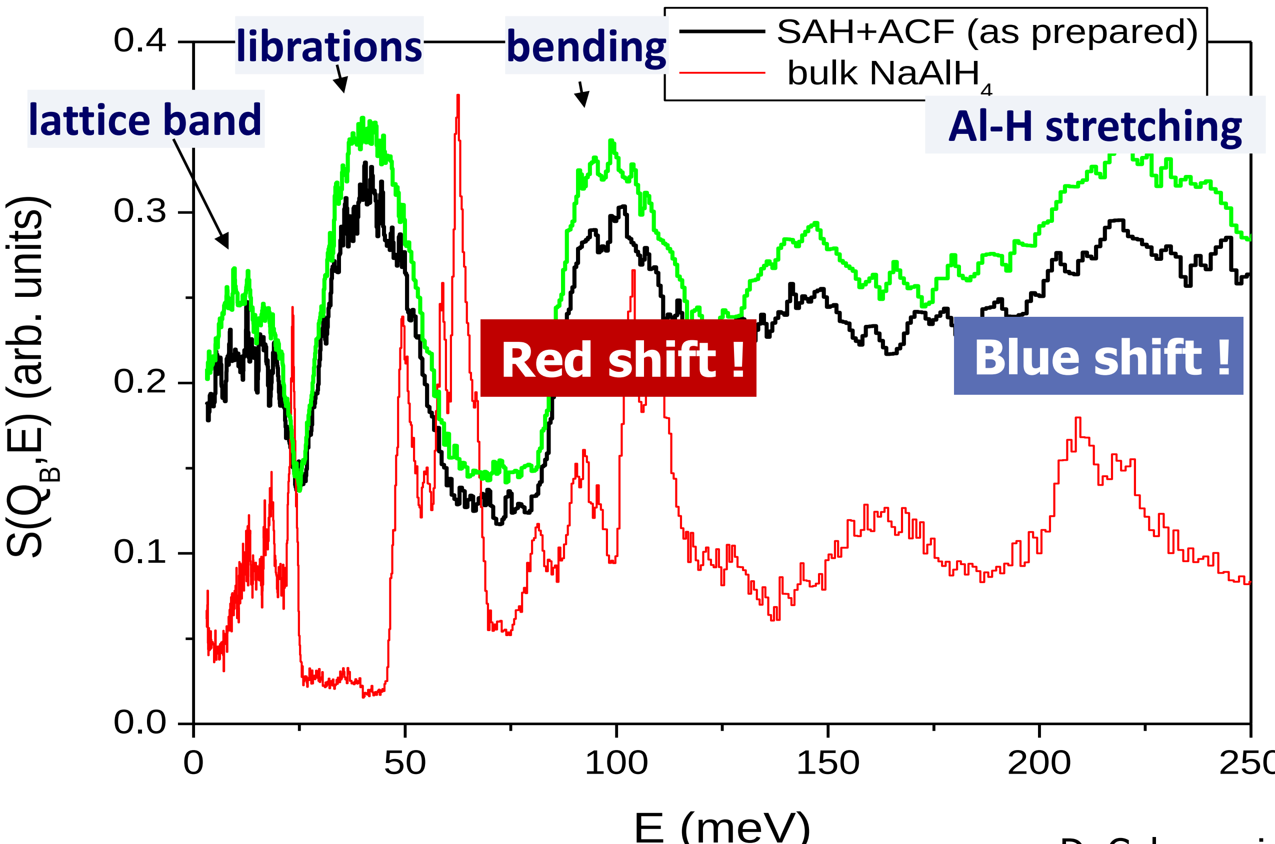
Matches predictions of our theorists (UniO).

Zhao-Karger *et al.*, Chem.Comm. (2010)

Results

Mechanistic understanding

Vibrational properties → INS, Raman



First INS study on nanoconfined hydrides.

Explanation of macroscopic behaviour.

Matches the predictions made by our theoreticians (UniO).

D. Colognesi *et al.*, J. Phys. Chem. C (2011)

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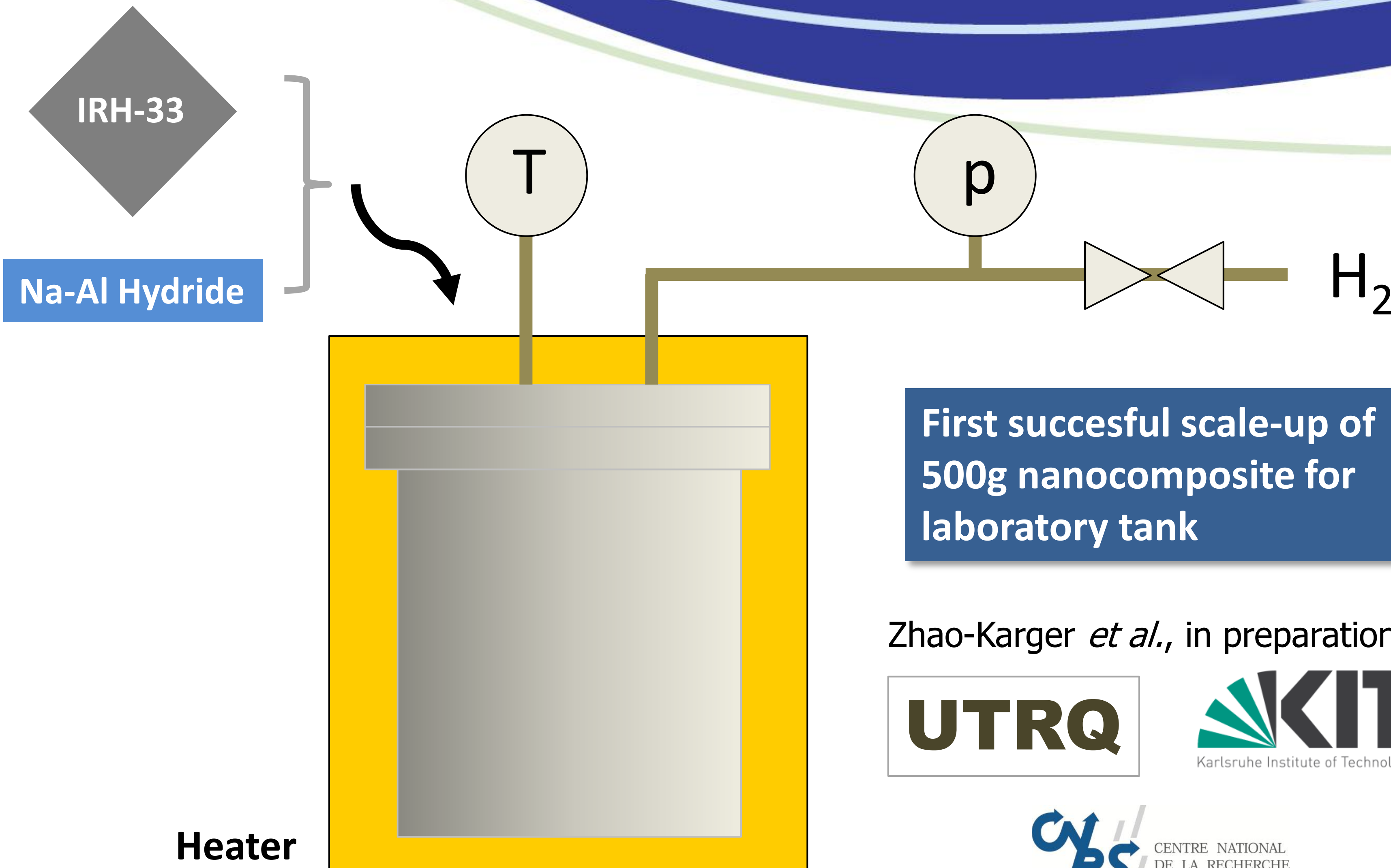
Results



First succesful scale-up of 500g nanocomposite for laboratory tank

Zhao-Karger *et al.*, in preparation

UTRQ

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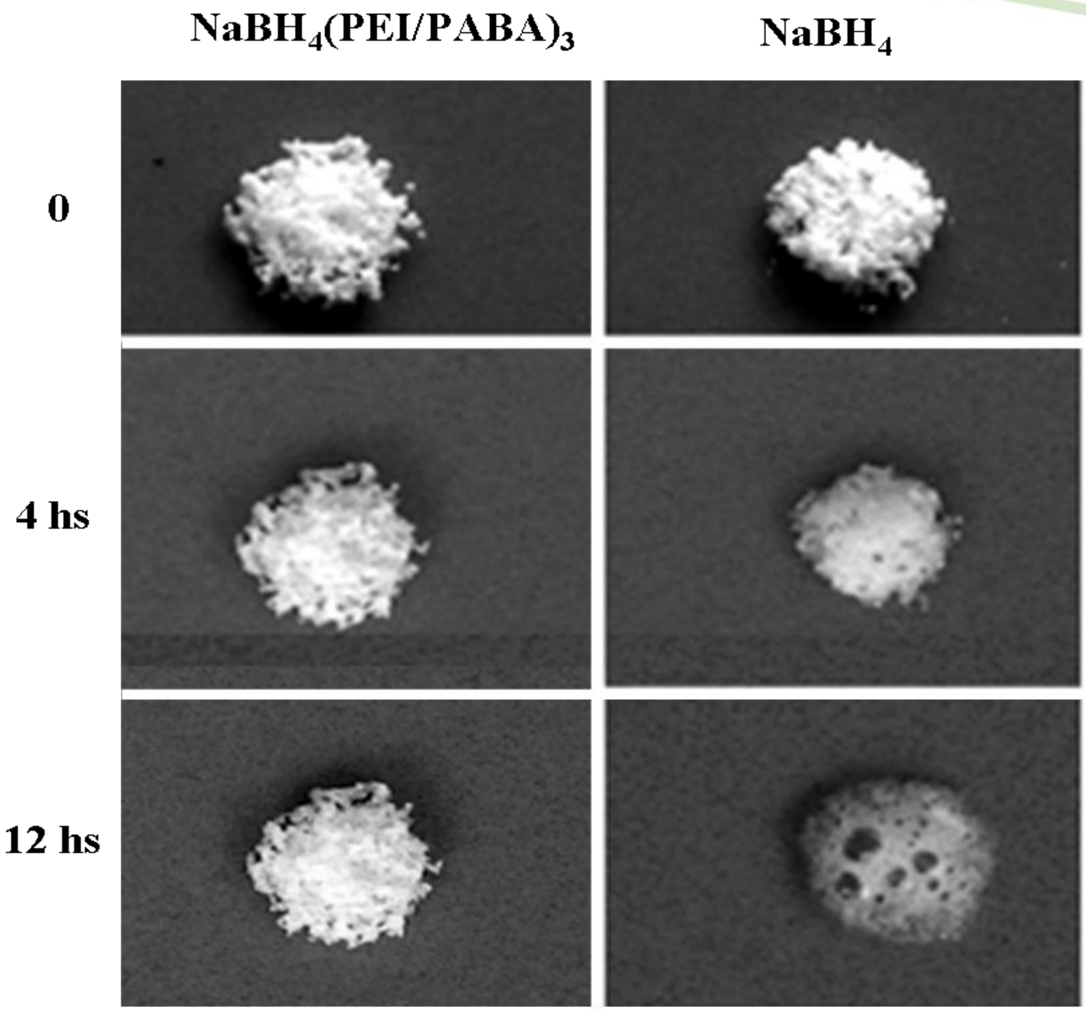
Results

Safety



First self-assembled and stable nanocoating of complex hydrides

→ Reactivity in air reduced

T. Borodina *et al.*, J. Mater. Chem (2010)

Max Planck Institute of Colloids and Interfaces

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Project activities/results versus MAIP/AIP targets:

- ***Functional materials with altered thermodynamic and kinetic properties.***
- ***No catalyst needed for reversibility***
- ***Upscale of material is possible***

Gaps/bottlenecks :

- ***Development of composites with high gravimetric density.***
- ***Cost of raw materials.***
- ***Materials properties: microporous scaffolds with higher pore volume needed to increase storage capacity.***

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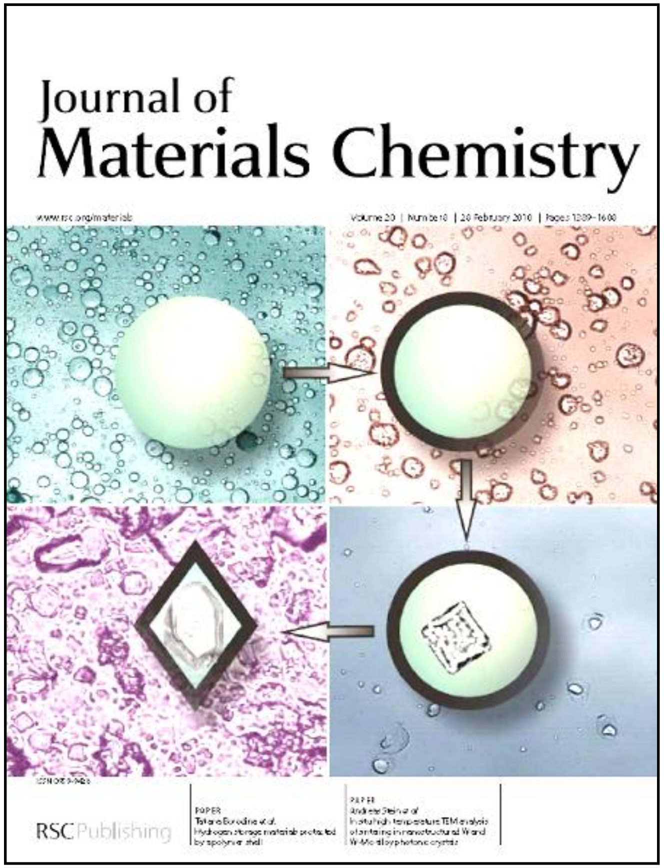
Cross cutting issues

- *Training: 3 students and 10 post docs (6 female) involved in the project*
- *Dissemination & public awareness : > 55 papers & conference contributions*
- *Two Workshops.*
- *Website www.nanohy.eu*
- *Succesful spin-off of infiltration technologies to battery technology.*



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Conclusion

- NANOHy has adressed several of the major problems of H storage.
- 9 partners from 6 different countries work on the encapsulation of complex hydrides at the lower nanoscale, the modelling and characterization of such materials and on their system integration.
- International leading activity.
- It is possible to infiltrate microporous scaffolds by complex hydrides and change their properties: Considerable improvement of kinetics observed. Thermodynamic effects were observed for the first time. Property changes were succesfully predicted by modeling.
- Not possible: change of the reaction path so that irreversible bulk hydrides become reversible → no improvement of reversible storage capacities by using these hydrides.
- Reactivity in air can be lowered by nanocoatings.
- First upscale production and lab tank development with hydride/AC composite.
- Spin off to other functional materials.

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Perspectives

- NANOHy work has been done in close relation to IP NESSHy and several national activities (FuncHy, NANOMAT etc.).
- Most of the NANOHy partners are experts/representatives at the IEA-HIA Task 22 → close collaboration at the highest level with other international activities.
- Further development of scaffolds (and hydrides) is necessary to improve storage capacity.
- Ongoing spin-off of knowledge to other functional materials.
- Proposals on new functional materials (e.g. batteries) in upcoming EC calls.
- Already contacts to potential partners of a future consortium.

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Acknowledgments

Thank you for your attention

:FutureCarbon

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