Bor4store @ UNITO

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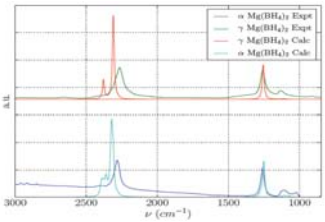
Introduction:

In the framework of the BOR4STORE project UNITO is leader of WP3, based on *ab initio* calculations, thermodynamic and kinetic modelling. For a modern scientific approach the combination of experiments with modelling techniques is extremely important, indeed the use of models allows a pretty fast and cheap screening of possible candidate materials and its combination with experiments provides a deeper understanding of the material properties.
Moreover in WP1 and WP2, UNITO is involved for the experimental characterization of selected materials.

Modelling

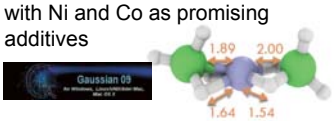
Ab initio

Thermodynamics: reactions and stability of different polymorphs *(inputs for TD modelling)*

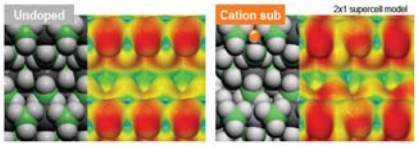


IR spectra *(comparison with experiments)*

Exploring reactivity of $M(BH_4)_n$ with Ni and Co as promising additives

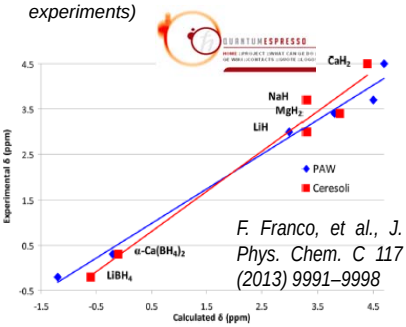


Effect of additives inclusion of Ni,Co,Cu,Zn on $Mg(BH_4)_2$ and $Ca(BH_4)_2$ model surfaces



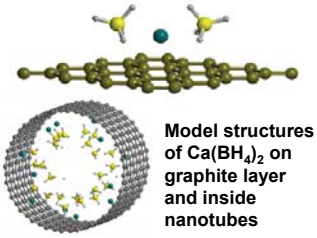
$Mg(BH_4)_2$ - *010*

NMR spectra *(comparison with experiments)*



F. Franco, et al., J. Phys. Chem. C 117 (2013) 9991–9998

Scaffolding of $M(BH_4)_n$ (M=Li,Ca,Mg) in nanotubes and graphene: mainly a size effect



Model structures of $Ca(BH_4)_2$ on graphite layer and inside nanotubes

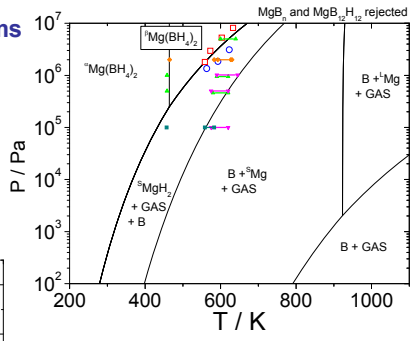
CALPHAD

Borohydrides phase diagrams

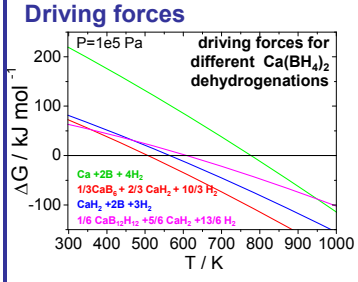
Assessed functions for **$M(BH4)_n$** (M=Li,Na,K,Mg,Ca) and **$M_nB_{12}H_{12}$** (M=Li,Na,Mg,Ca)

E.R. Pinatel et al., JALCOM s645 (2015)S64–S68.

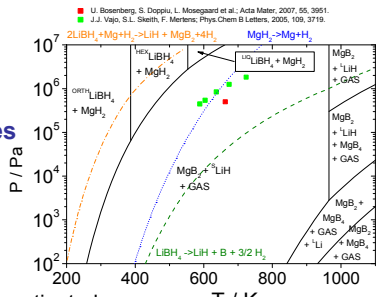
T vs. P phase diagram for $Mg(BH_4)_2$



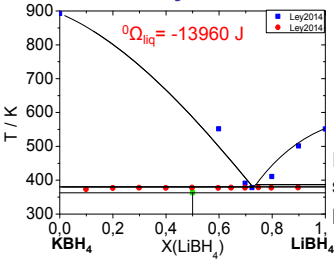
Driving forces



Reactive Hydrides Composite



Eutectic borohydrides mixtures



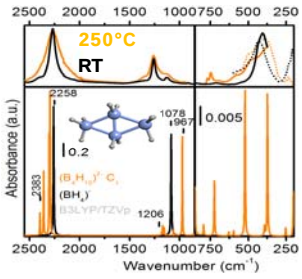
Investigated systems: Li-Na, Li-K, K-Na

$2LiBH_4$+MgH_2 *(Input for tank design)*

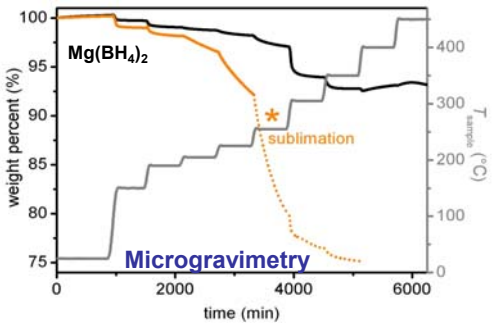
Experiments

IR spectroscopy

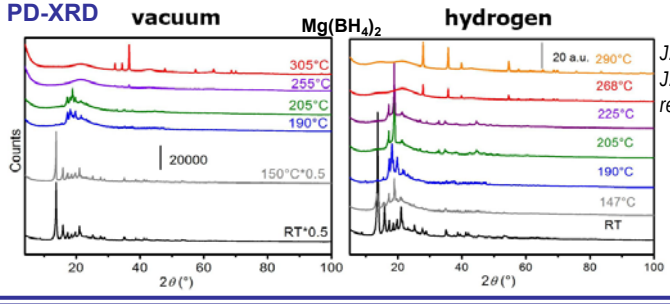
Comparison between experimental and ab initio calculated spectra to identify intermediates of the $Mg(BH_4)_2$ dehydrogenation reaction



Characterization of the different dehydrogenation paths of **$Mg(BH_4)_2$ based samples** *in vacuum and hydrogen atmosphere by:* **PCI, Microgravimetry, ATR-IR, UV-Vis, XRD**)



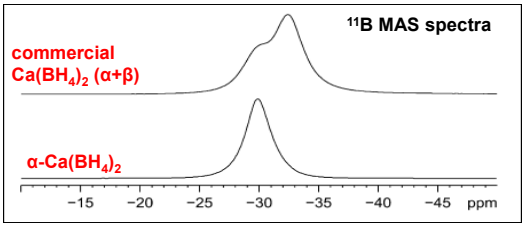
PD-XRD



J. G. Vitillo, et al., J. Phys. Chem. C revised (2015).

SS-NMR

LiH, NaH, CaH_2, MgH_2, $LiBH_4$, $NaBH_4$, $Ca(BH4)_2$, $Na_2B_{12}H_{12}$, $K_2B_{12}H_{12}$



Conclusions

- Experiments and modelling have been successfully coupled to reach a deeper understanding
- Effect of additives and infiltration in porous scaffolds has been investigated
- A consistent thermodynamic database for hydrides and borohydrides has been developed
- Key experiments have been performed to understand $Mg(BH_4)_2$ dehydrogenation path
- A systematic SS-NMR study for hydrides, borohydrides and closoboranes has been carried out

Acknowledgements

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