



Controlling the synthesis of superior MgH₂ nanostructures for hydrogen storage



UNSW AUSTRALIA

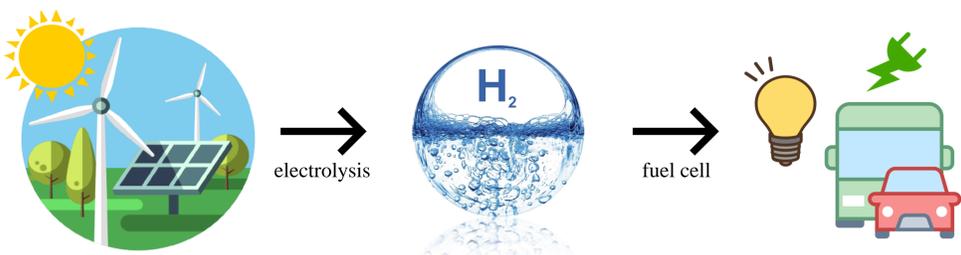
Nigel Rambhujun, Kondo-Francois Aguey-Zinsou
MERLIN, School of Chemical Engineering, University of New South Wales, Australia

Introduction

Hydrogen – the fuel of the future?

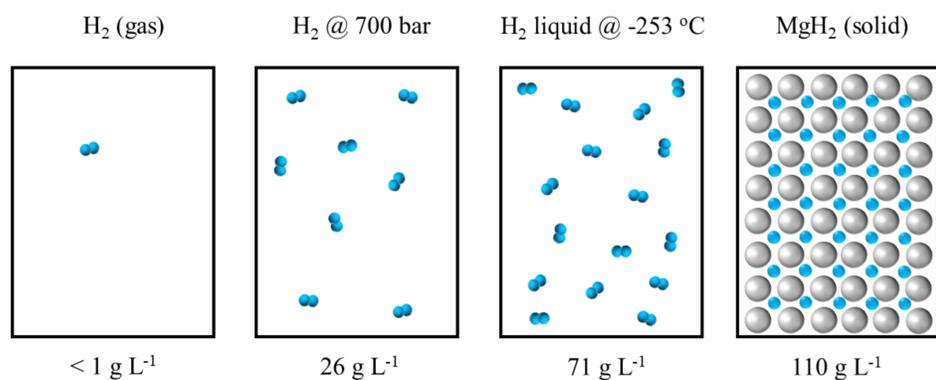
Recently, green hydrogen (produced from renewable energy sources) has received significant interest as a clean and sustainable energy solution to address the net-zero emissions goal due to:

- High energy density (120 MJ kg⁻¹ for hydrogen vs. 45 MJ kg⁻¹ for gasoline)
- Non-polluting and environmentally friendly (main product of combustion is H₂O)
- Abundant and regenerative (can be produced directly by splitting water)
- Flexible uses (fuel for transportation, generation of electricity and heat)



Motivation

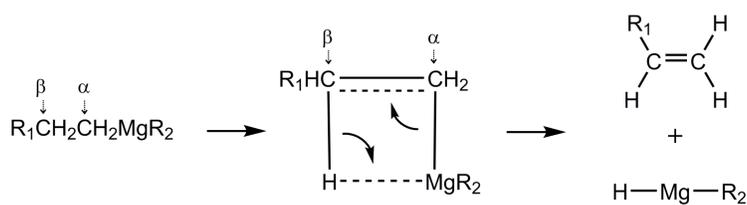
The storage and transportation of hydrogen is **challenging** due to its low boiling point (-253 °C) and low volumetric density (0.089 g L⁻¹). Novel hydrogen storage methods are thus being developed such as solid-state storage in magnesium hydride (MgH₂) due to its **high volumetric density** (110 g L⁻¹) and **gravimetric density** (7.6 mass% H₂).



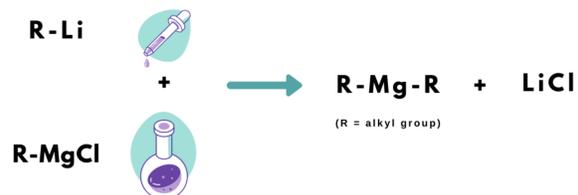
Unfortunately, MgH₂ suffers from **poor thermodynamics** and **kinetics**, resulting in a high H₂ desorption temperature (> 300 °C) and slow H₂ absorption/desorption. In this work, we attempted to improve the hydrogen storage properties by controlling the synthesis of MgH₂.

Synthesis Approach

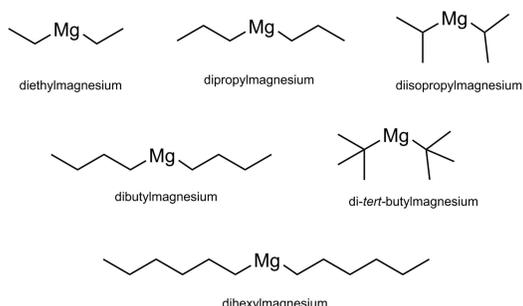
MgH₂ can be synthesised from the thermal decomposition of Grignard reagents (e.g. bu₂Mg).



By controlling the type of Grignard reagent used, it should be possible to control the MgH₂ synthesis.

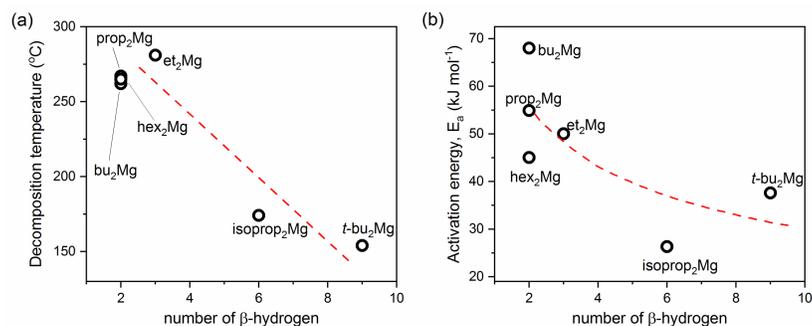


Six different halide-free Grignard reagents were prepared, with differences in their carbon chain length and number of β-hydrogen, and their decomposition behavior investigated.

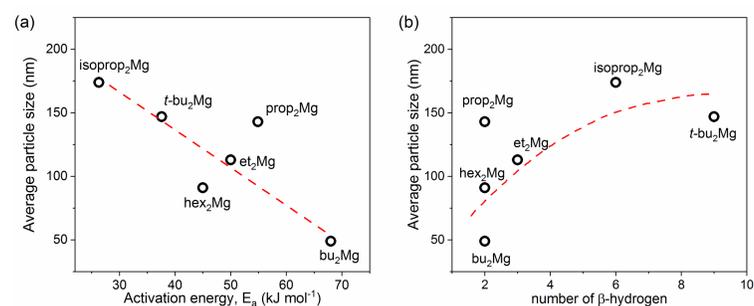
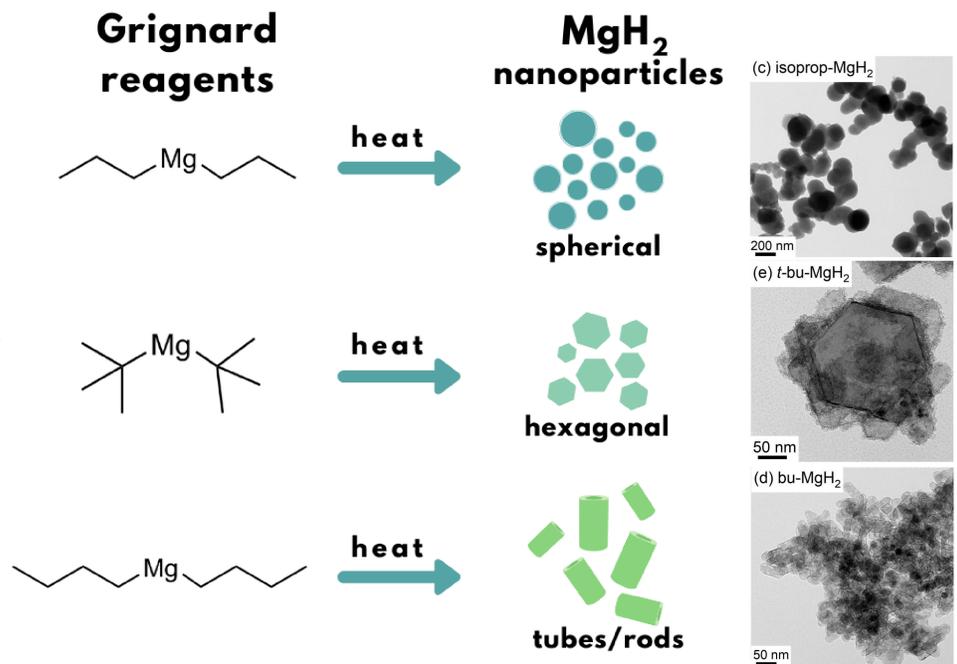


Key Findings

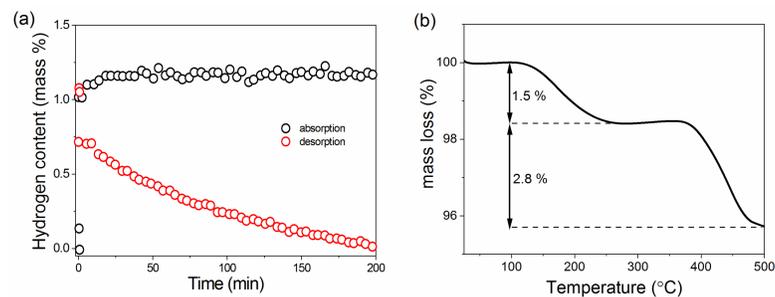
A correlation was observed when plotting (a) the decomposition temperature and (b) the activation energy of the Grignard reagents as a function of the number of β-hydrogens.



Following the thermolysis of the Grignard reagents at 260 °C, different morphologies and particle sizes were obtained from the organomagnesium precursors.



Further investigations of *t*-bu₂Mg revealed that hydrogen release from MgH₂ occurred as early as 130 °C.



Conclusion

- The stereochemistry & chain length of Grignard reagents influenced their decomposition.
- The choice of Grignard reagents affected the size and morphology of MgH₂ nanoparticles.
- Di-*tert*-butylmagnesium had the lowest decomposition temperature, and its thermolysis generated MgH₂ particles that had an early hydrogen release due to metastable γ-MgH₂.

Bibliography

1. Rambhujun, N. & Aguey-Zinsou, K.-F., (2021). Halide-free Grignard reagents for the synthesis of superior MgH₂ nanostructures. International Journal of Hydrogen Energy, 46(56)
2. Rambhujun, N., Salman, M. S., Wang, T., Prathana, C., Sapkota, P., Costalin, M., & Aguey-Zinsou, K.-F. (2020). Renewable hydrogen for the chemical industry. MRS Energy & Sustainability, 7(1)