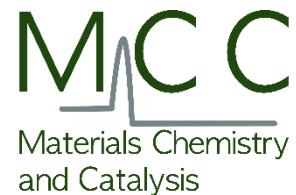




**Utrecht  
University**



**Debye Institute for  
Nanomaterials Science**

# Metal Hydride nanocomposites as transition metal free catalysts for ammonia synthesis

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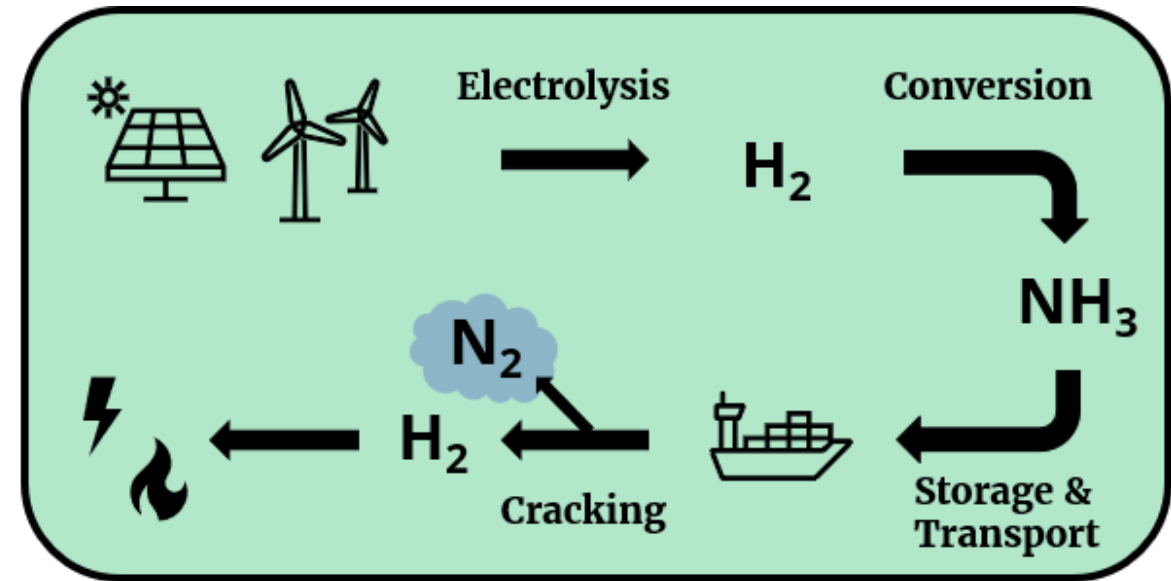
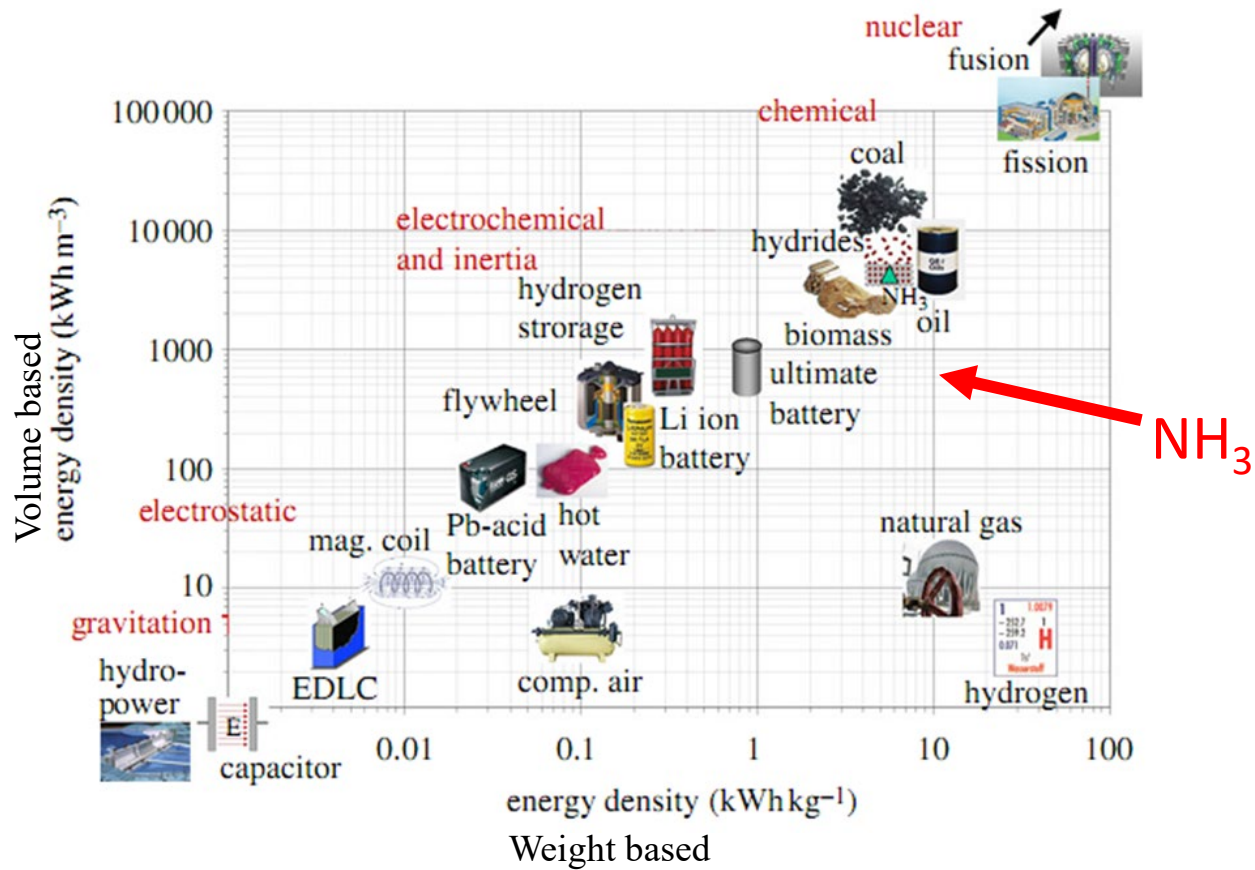
*10<sup>th</sup> of June 2025*

*NAM29, Atlanta GA*



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# Ammonia as an energy carrier



Ammonia is increasingly recognized as a highly viable chemical energy carrier.

# Ammonia synthesis



For high ammonia yield: low temperature and high pressure  
(from thermodynamics)

For fast ammonia formation: high temperature  
(from kinetics)

**Catalysts**

**Efficient ammonia production**  
Reaction at temperatures as low as possible

# Ammonia synthesis catalysts

~ consumes 2% global energy production



**Haber-Bosch process  
(Fe based catalyst)**

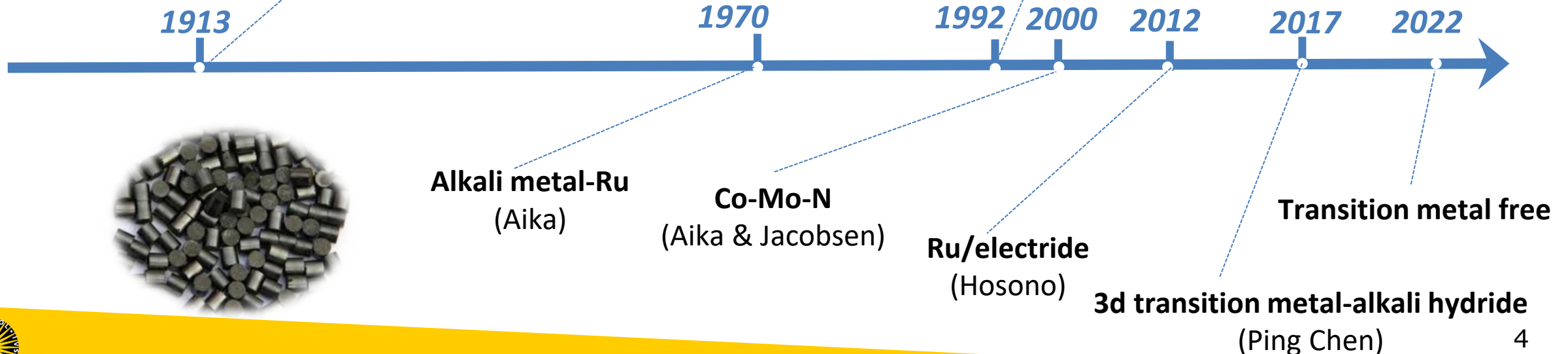
1<sup>st</sup> generation  
(Haldor Topsoe)  
 $\text{Fe}_3\text{O}_4 + \text{Al}_2\text{O}_3 + \text{K}_2\text{O} + \text{CaO}$   
350-525 °C, 100-300 bars

525 to 325 °C

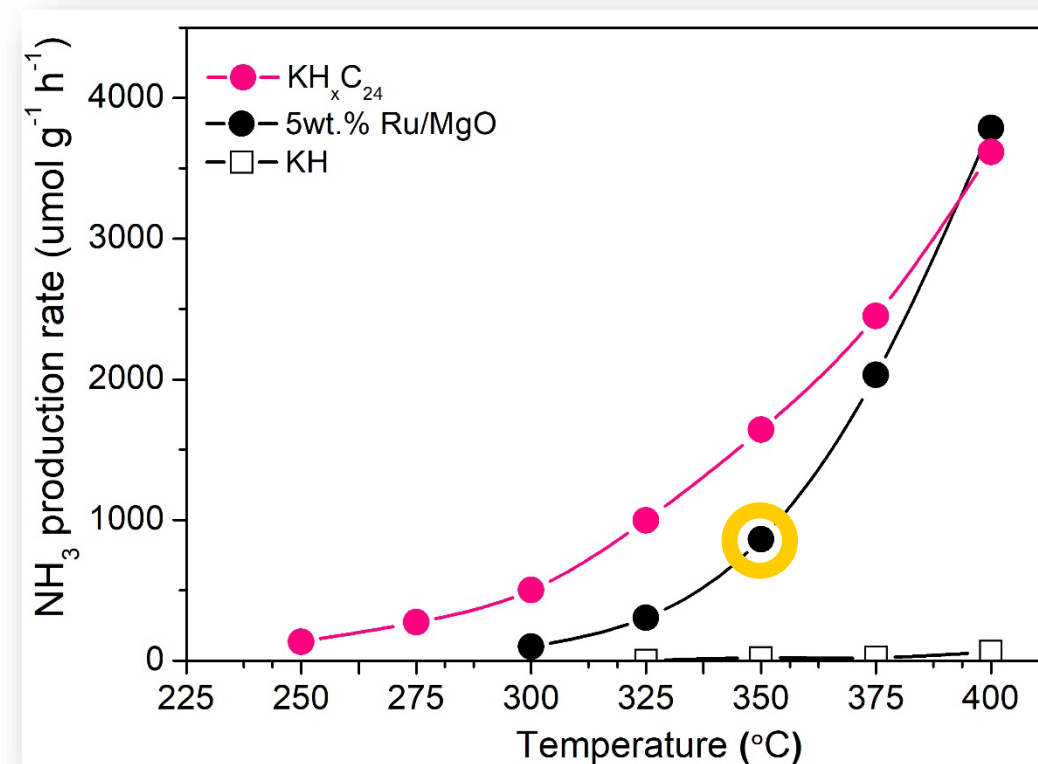
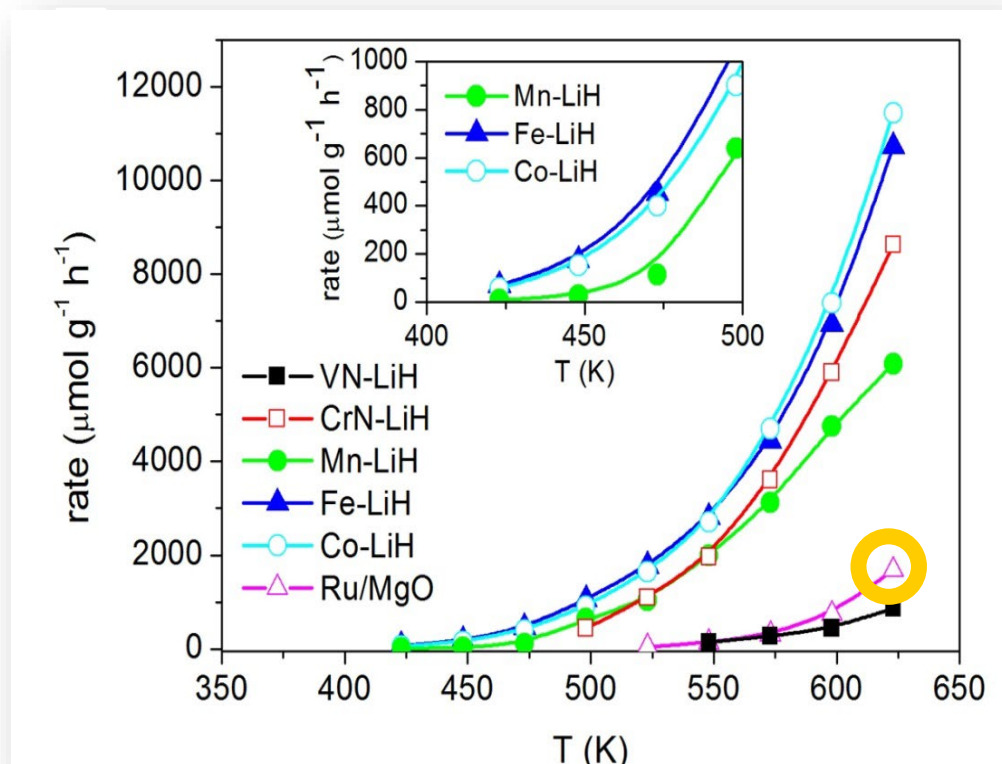
350 to 100 bar

**KAAP Process  
(Ru based catalyst)**

2<sup>nd</sup> generation  
(BP)  
Ru-Ba-K/AC  
325-450 °C, ≤ 100 bars



# Alkali hydride mediated ammonia synthesis



- 3d TM+LiH composite catalysts achieved ammonia synthesis at a temperatures as low as 150°C
- KHC nanocomposites catalysts achieved ammonia synthesis at temperatures as low as 250°C

NH<sub>3</sub> synthesis catalyzed by different catalysts under the conditions of 1 MPa, 1N<sub>2</sub>:3H<sub>2</sub> and flow rate = 60,000 (left) – 36,000 (right) mL g<sub>cat</sub><sup>-1</sup> h<sup>-1</sup>.

# Alkali hydride mediated ammonia synthesis

Are other alkali metal (hydride) carbide nanocomposites also active for ammonia synthesis?

How does the ratio between alkali metal hydride and iron affect the catalytic activity?



# Alkali hydride carbide: ball milling

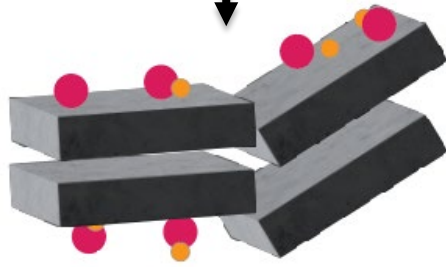
● K<sup>+</sup>  
● H<sup>-</sup>



Turbostratic graphite (C) +  
Potassium hydride (KH)

Ball Milling

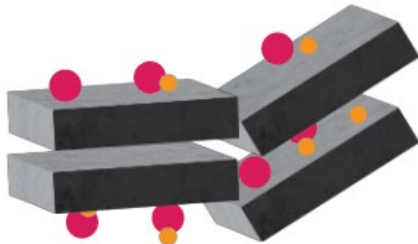
500rpm, 6h, 20:1



KH/C

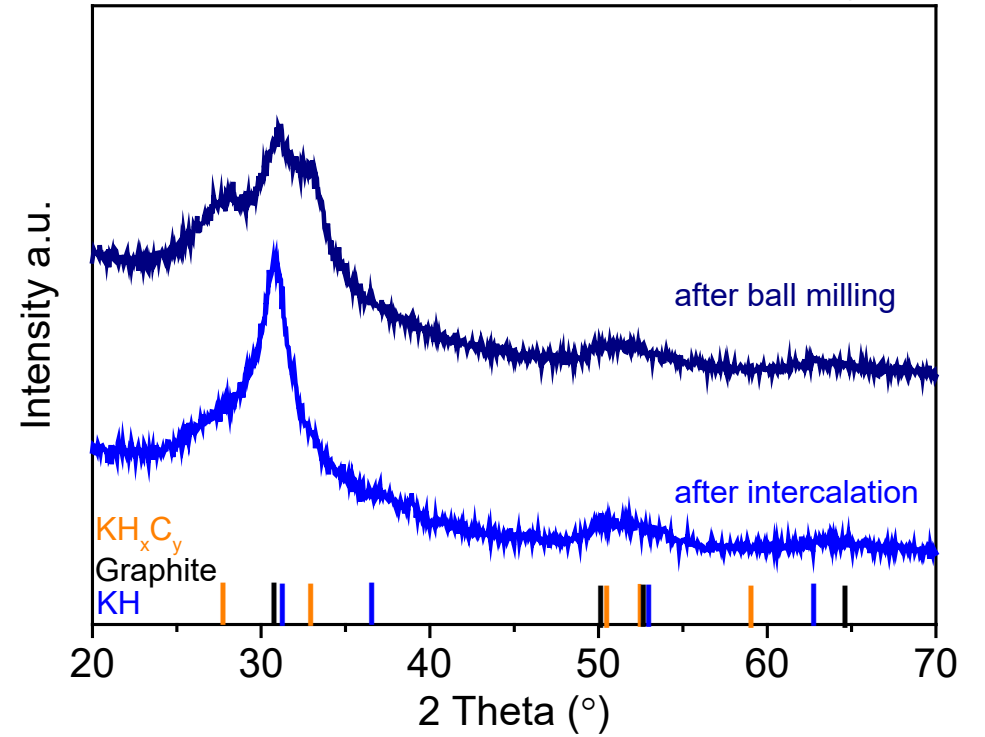
Heat treatment

(400°C, Ar, 2h)

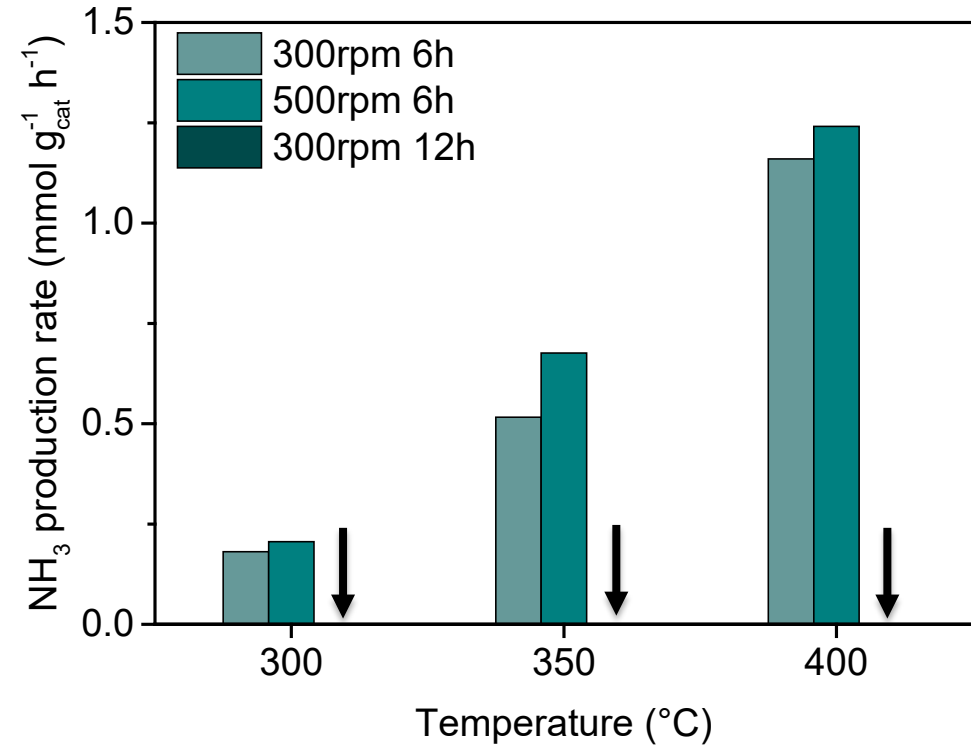
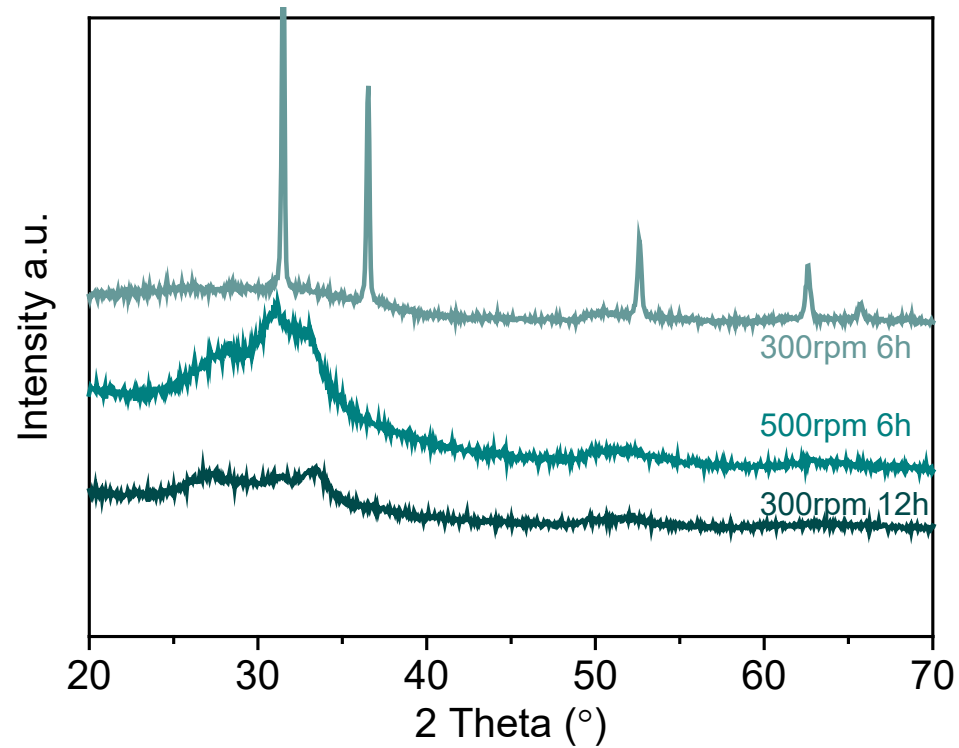


KH<sub>x</sub>C<sub>y</sub>

20wt% KH/C - 500rpm ball milling

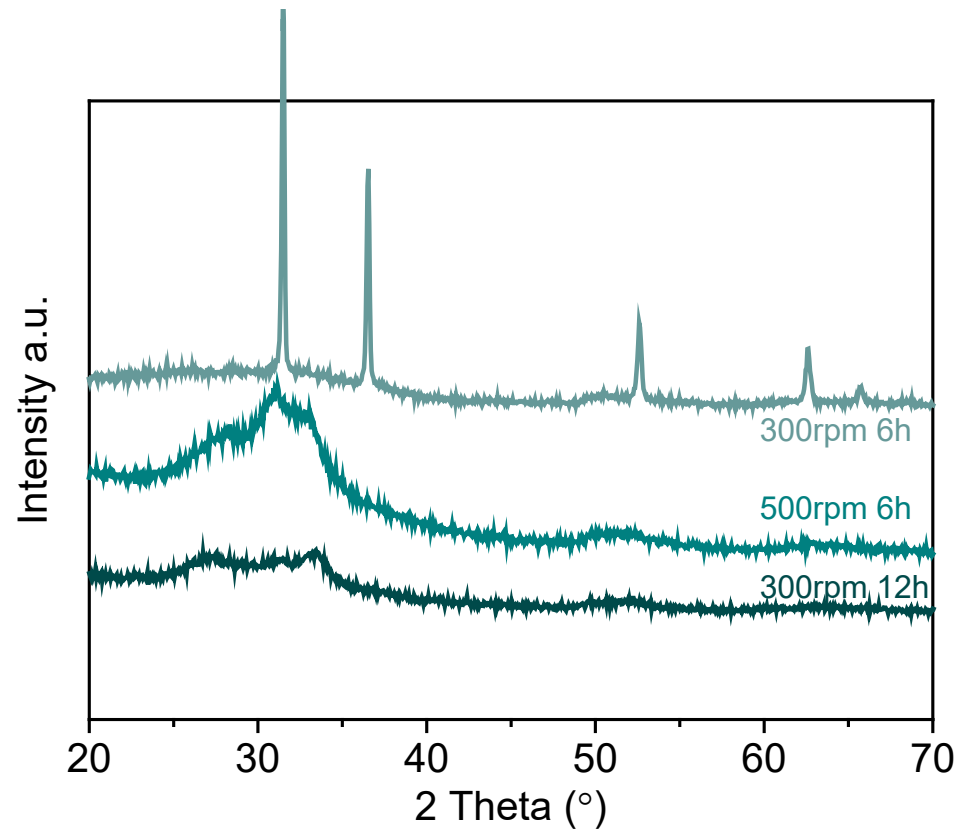


# KH-C: BM effect on 20wt%KH



BM can be used to synthesize KHC ammonia catalyst, but is prone to destruction

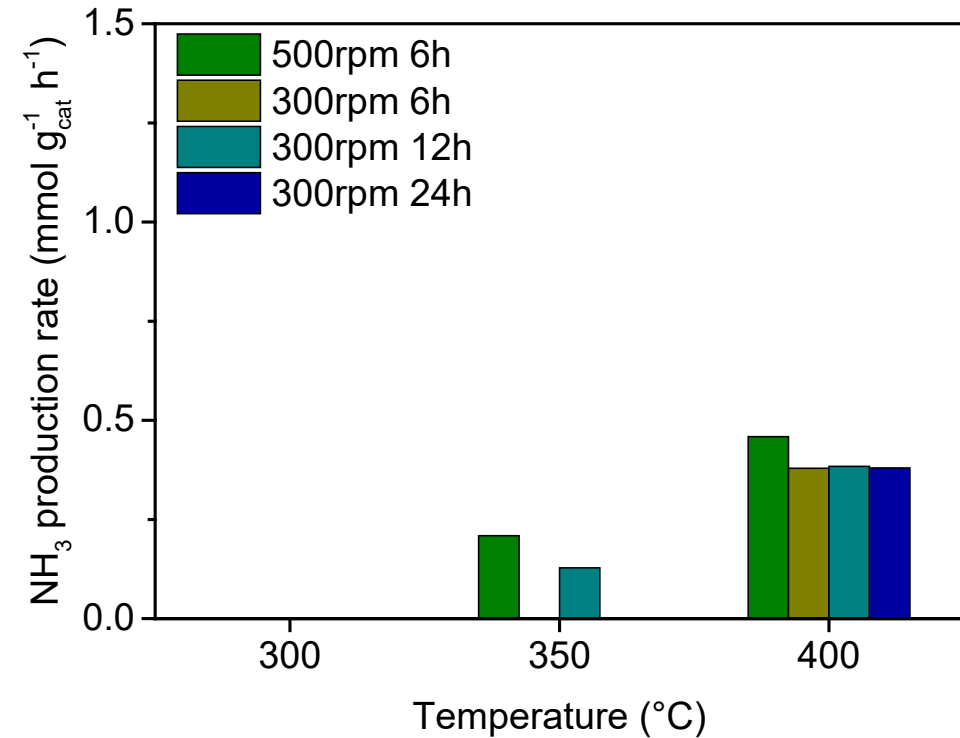
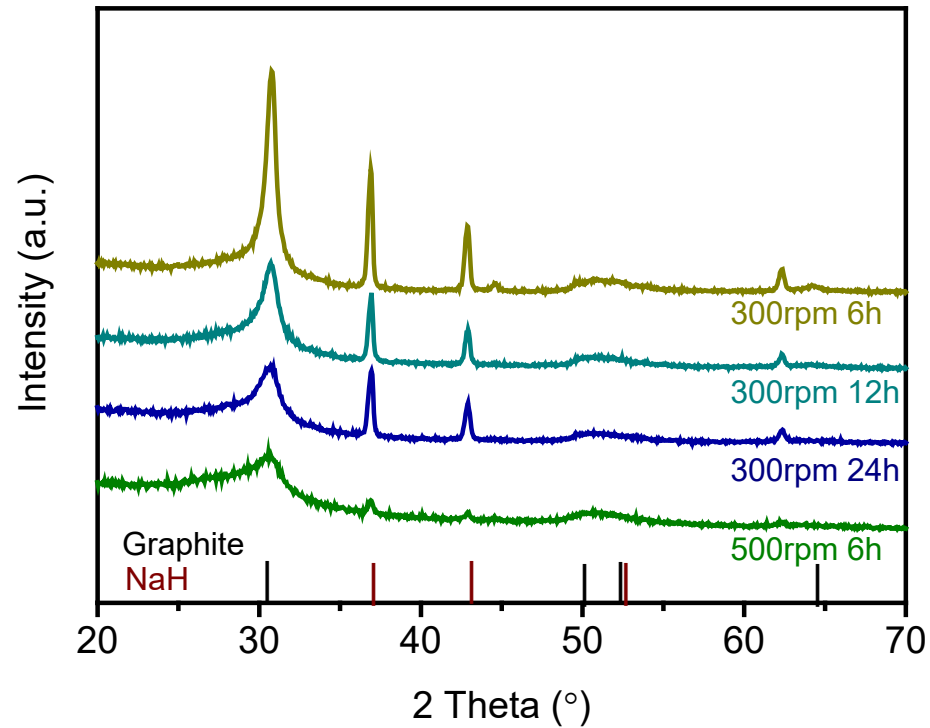
# KH-C: BM effect on 20wt%KH



BET SA (m <sup>2</sup> /g)	Pore volume (cm <sup>3</sup> /g)	NH <sub>3</sub> activity @400°C, 10 bar (mmol NH <sub>3</sub> g <sup>-1</sup> h <sup>-1</sup> )
238	0.26	1.16
9	0.02	1.24
75	0.09	0.00

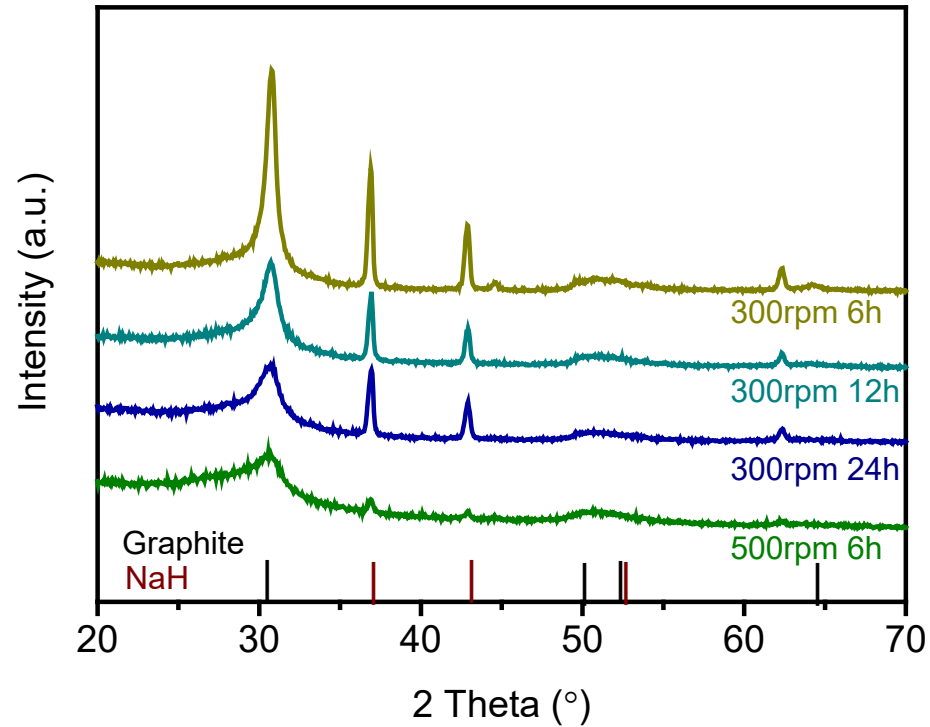
BM can be used to synthesize KHC ammonia catalyst, but is prone to destruction

# NaH-C: BM effect on 10wt%NaH



BM can be used to synthesize NaH/C ammonia catalyst, less prone to destruction in contrast to KHC

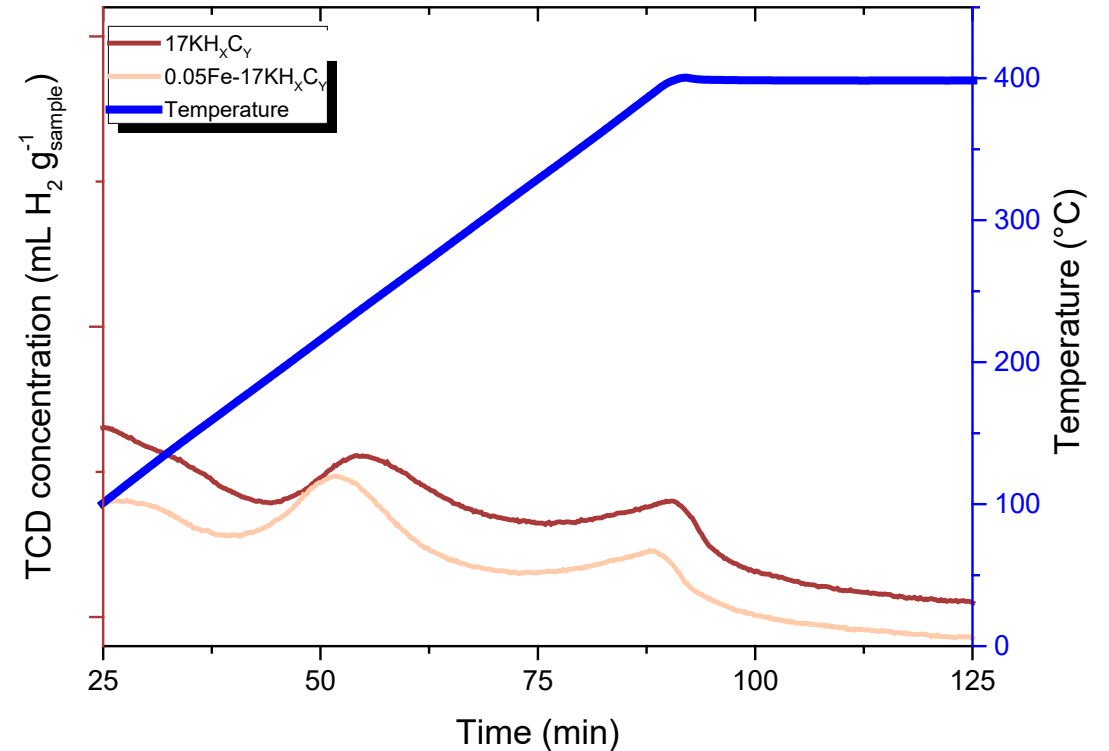
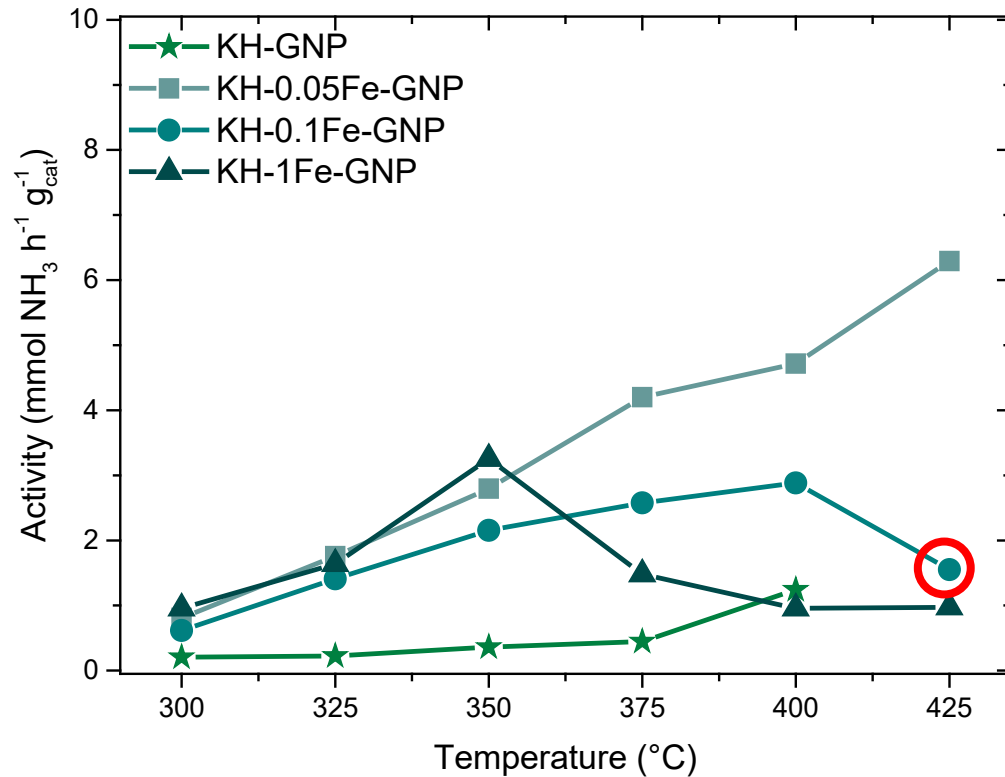
# NaH-C: BM effect on 10wt%NaH



BET SA (m <sup>2</sup> /g)	Pore volume (cm <sup>3</sup> /g)	NH <sub>3</sub> activity @400°C, 10 bar (mmol NH <sub>3</sub> g <sup>-1</sup> h <sup>-1</sup> )
452	0.67	0.38
477	0.52	0.38
542	0.66	0.33
360	0.33	0.46

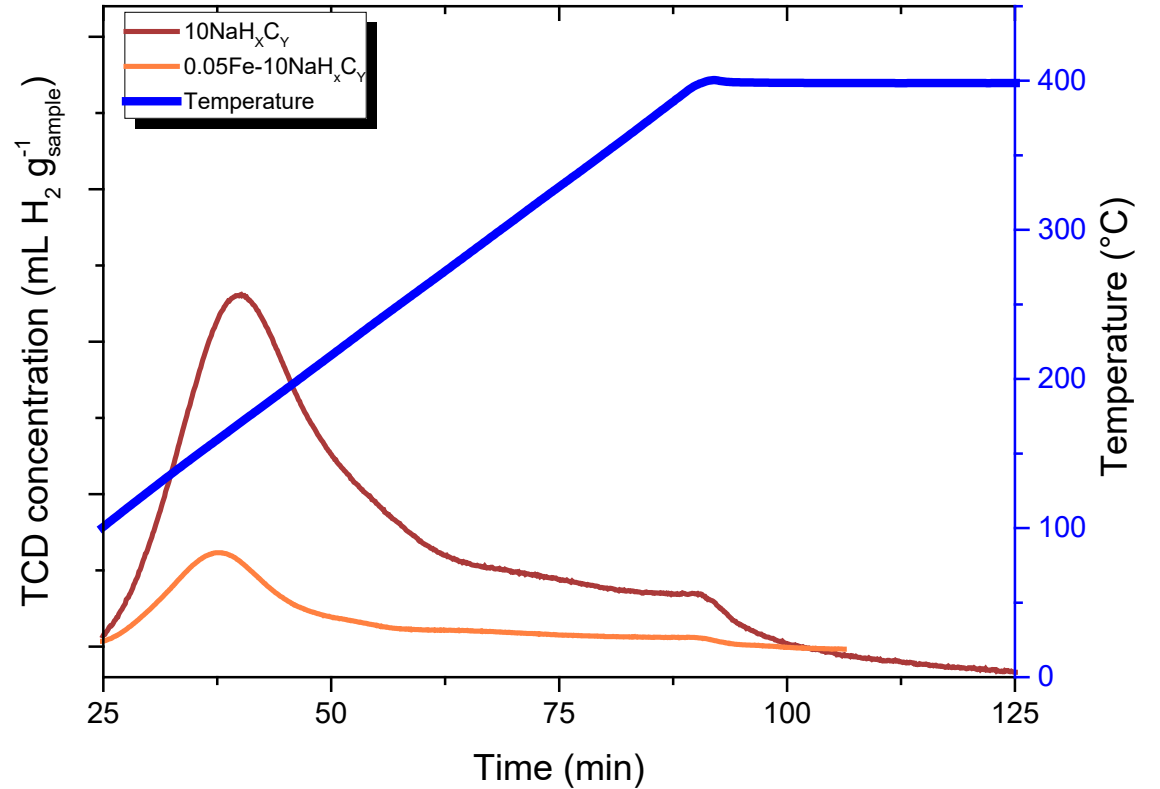
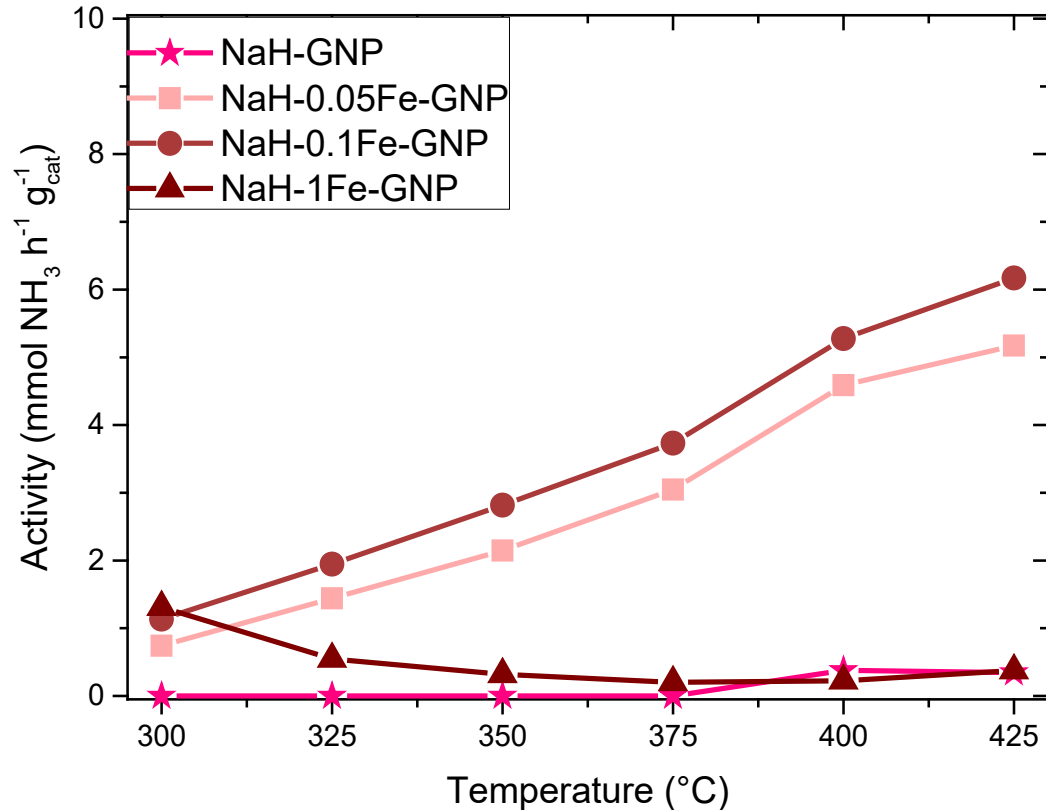
BM can be used to synthesize NaH/C ammonia catalyst, less prone to destruction in contrast to KHC

# Iron addition to alkali hydride



Addition of Fe increases activity, but the stability is very Fe-loading dependent

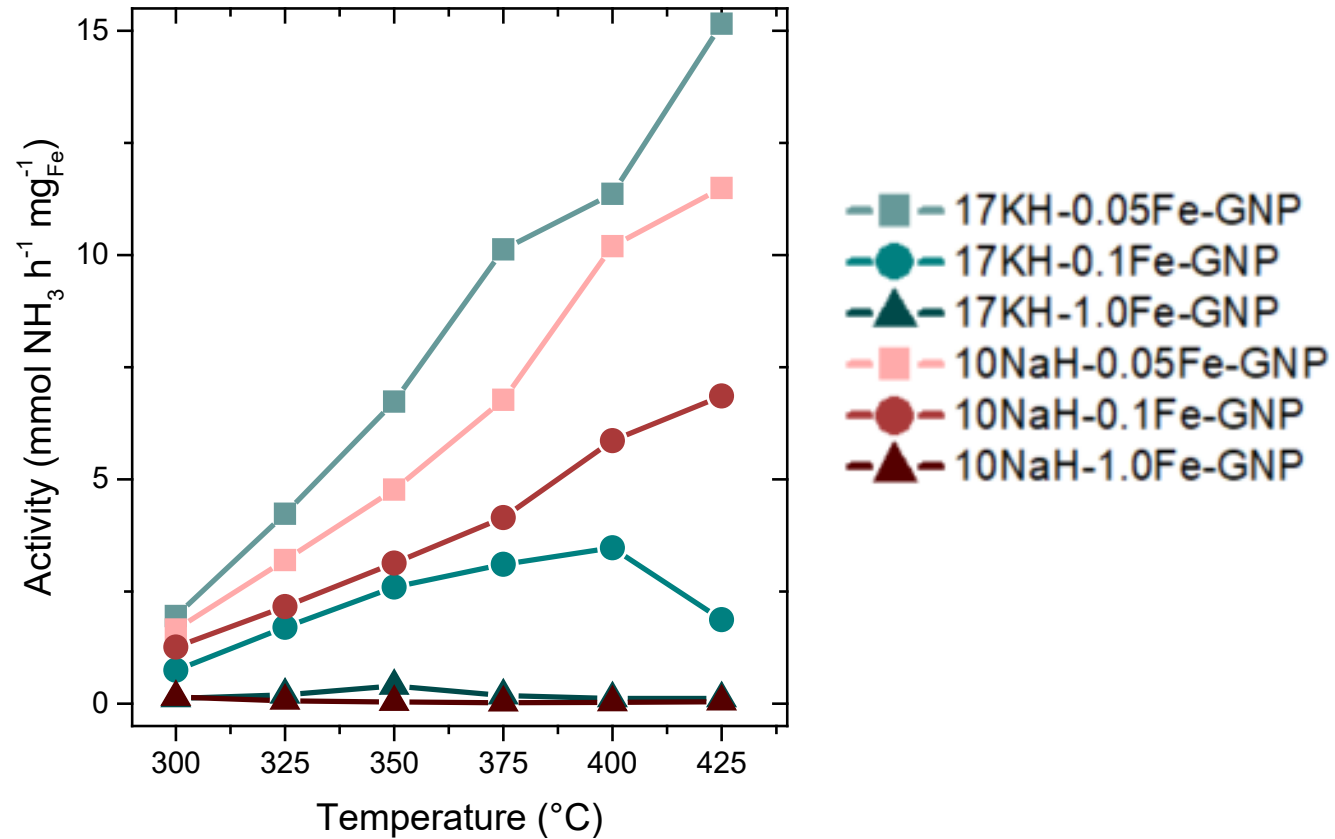
# Iron addition to alkali hydride



Addition of Fe increases activity, but the stability is very Fe-loading dependent



# Iron addition to alkali hydride



# Summarizing

1. Ball milling is a viable synthesis method for TM-free  $\text{NH}_3$  catalysts
2. Addition of Fe (<1wt%) increases the activity
3. Decreased Fe-loading result in increased stability



# Acknowledgements

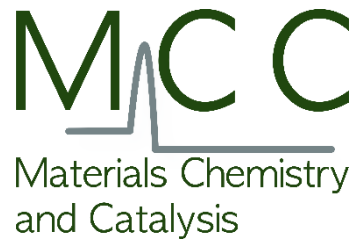
## Supervision

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*“Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union. Neither the European Union nor the granting authority can be held responsible for them.”*

