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MCC Materials Chemistry and Catalysis

Metal hydride nanocomposite materials as transition metal-free catalysts for ammonia synthesis

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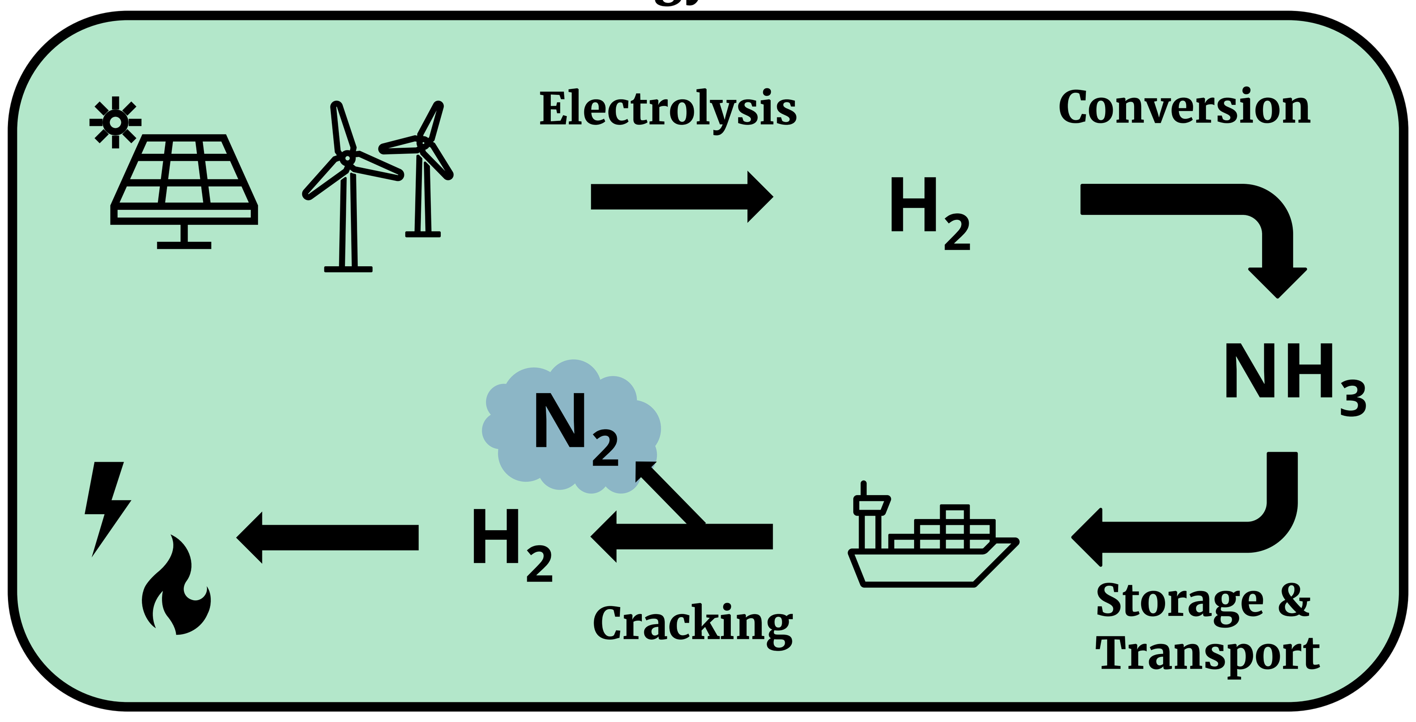
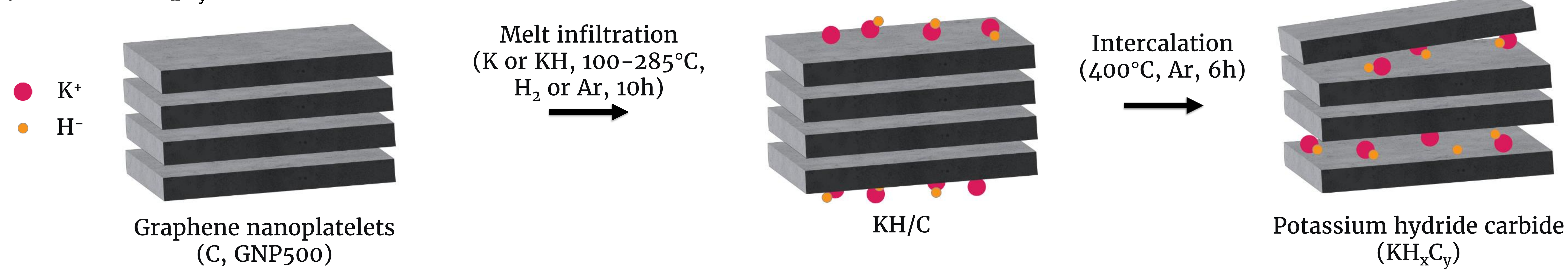
Introduction

Green hydrogen (H_2) produced from wind and solar can be used as a zero-emission fuel but has a low volumetric energy density and requires temperatures below -253°C to be liquified. Ammonia (NH_3) is a very important feedstock in the production of fertilizers, but over recent years has also emerged as a promising hydrogen carrier.[1] However, ammonia synthesis occurs at high temperatures and pressures, and accounts for 2% of the world energy consumption.[1] Consequently, there is a significant interest in developing novel catalysts that can activate nitrogen (N_2) at moderate temperatures, at which the equilibrium is more favorable.[2,3] Our study is focused on the synthesis, characterization and testing of transition metal-free catalysts, such as alkali hydride intercalated in graphitic carbon materials (AH_xC_y, A = Li, Na, K).

Renewable energy to carbon free fuels

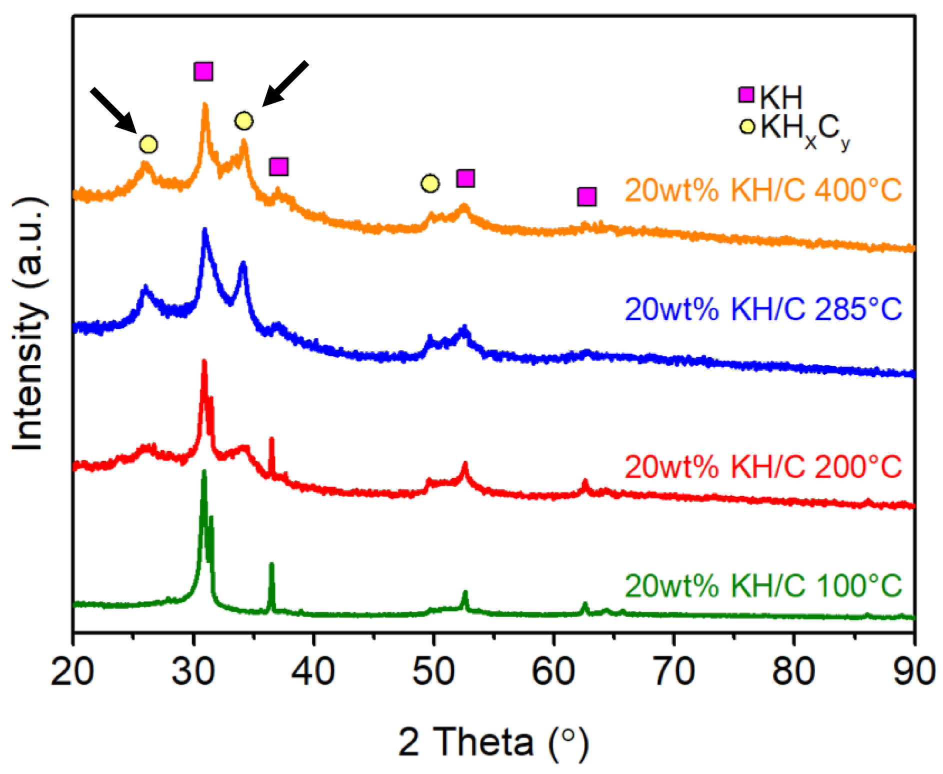


Synthesis of AH_xH_y, A = Li, Na, K



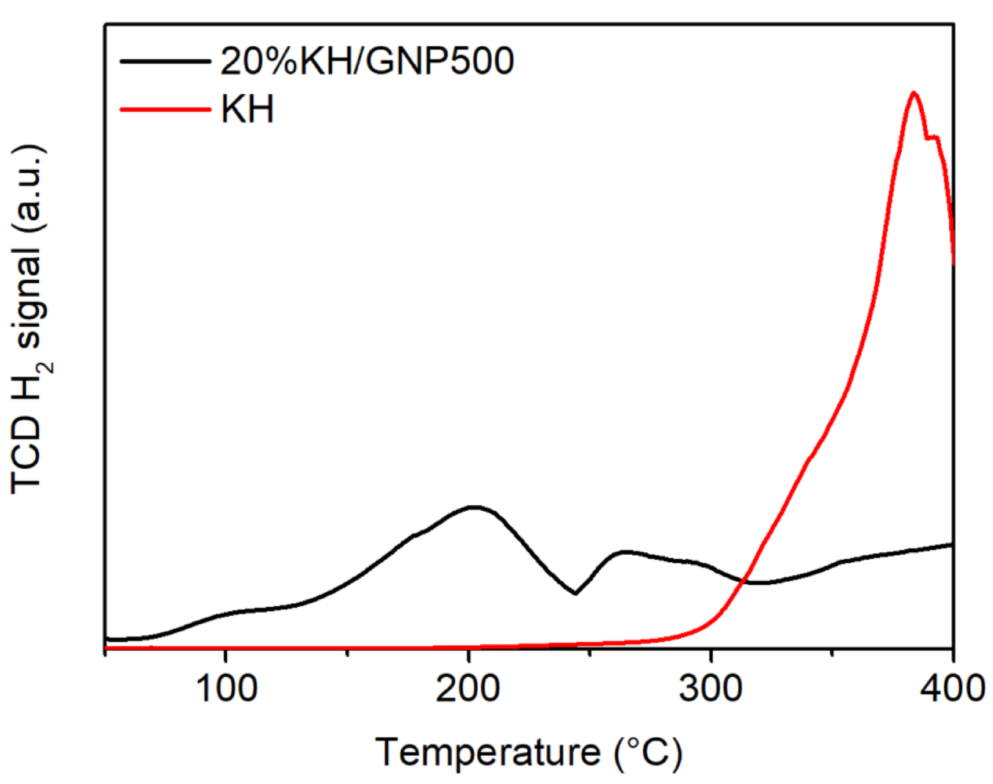
Synthesis: degree of intercalation

With increasing melt infiltration and intercalation temperatures the diffraction peaks attributed to the KH_xC_y phase appear more intensely.



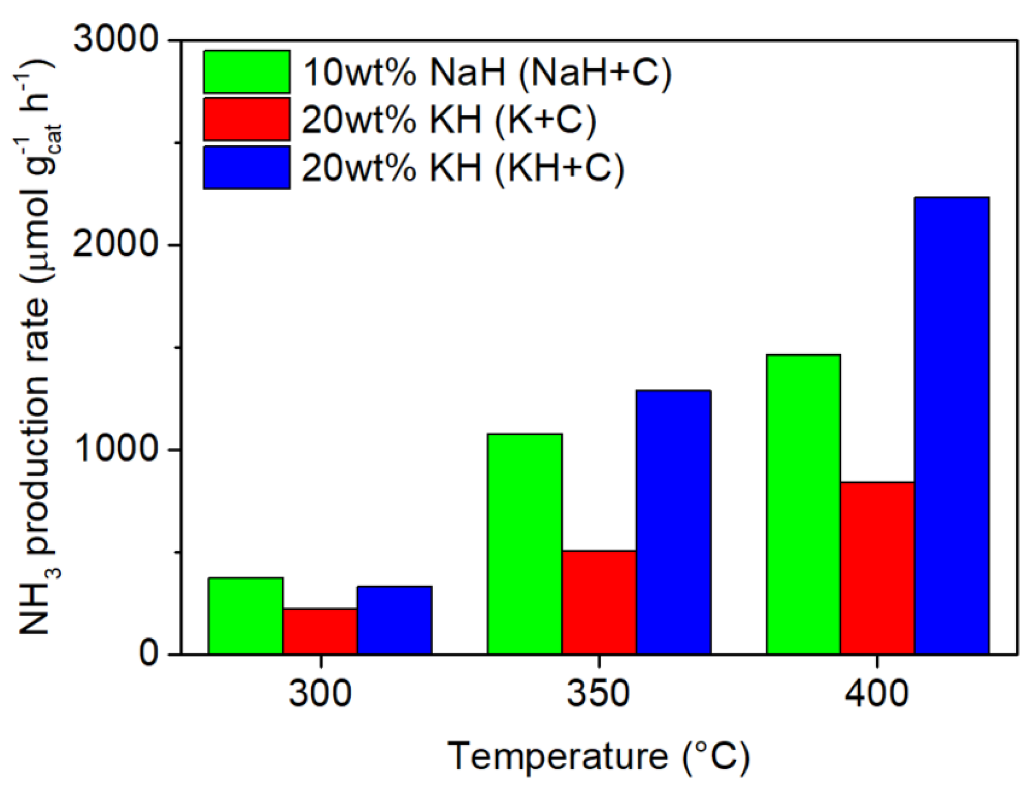
Synthesis: KH decomposition

TPD shows that during synthesis, partial decomposition of KH occurs in the presence of carbon, leading to KH_xC_y formation.



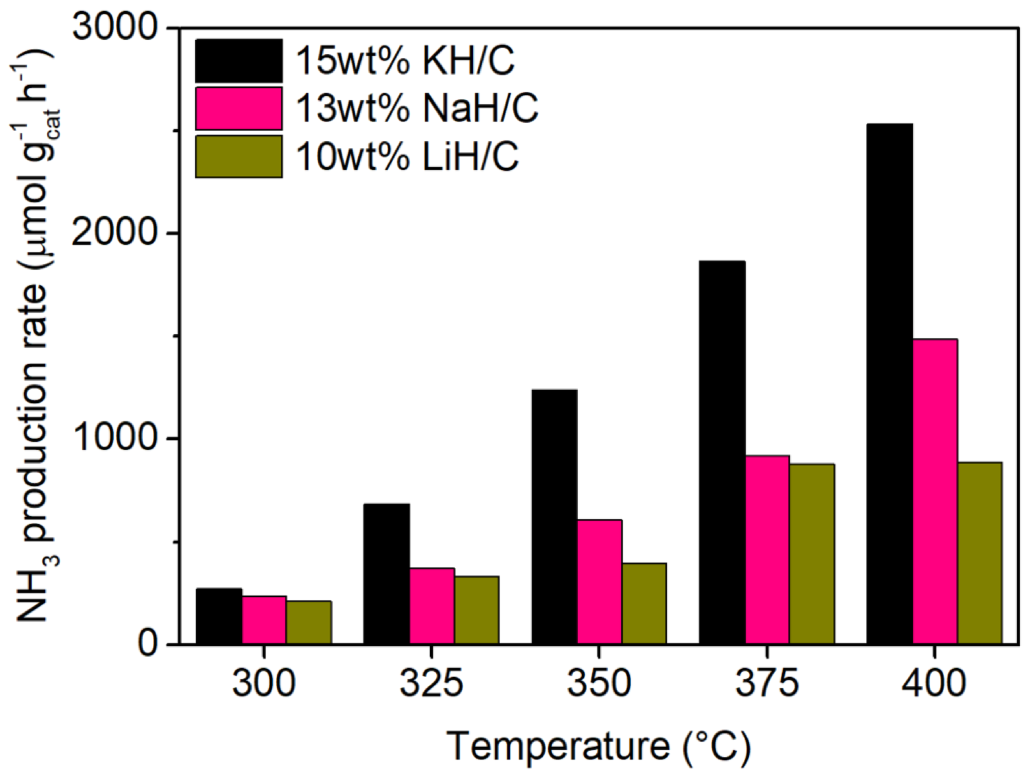
Catalytic activity: starting materials

The use of the hydride phase (KH) rather than the metallic phase (K) leads to much higher catalytic activity for ammonia synthesis.



Catalytic activity: alkali hydrides

We showed that different alkali hydrides (A = Li, Na, K) are active towards ammonia synthesis.

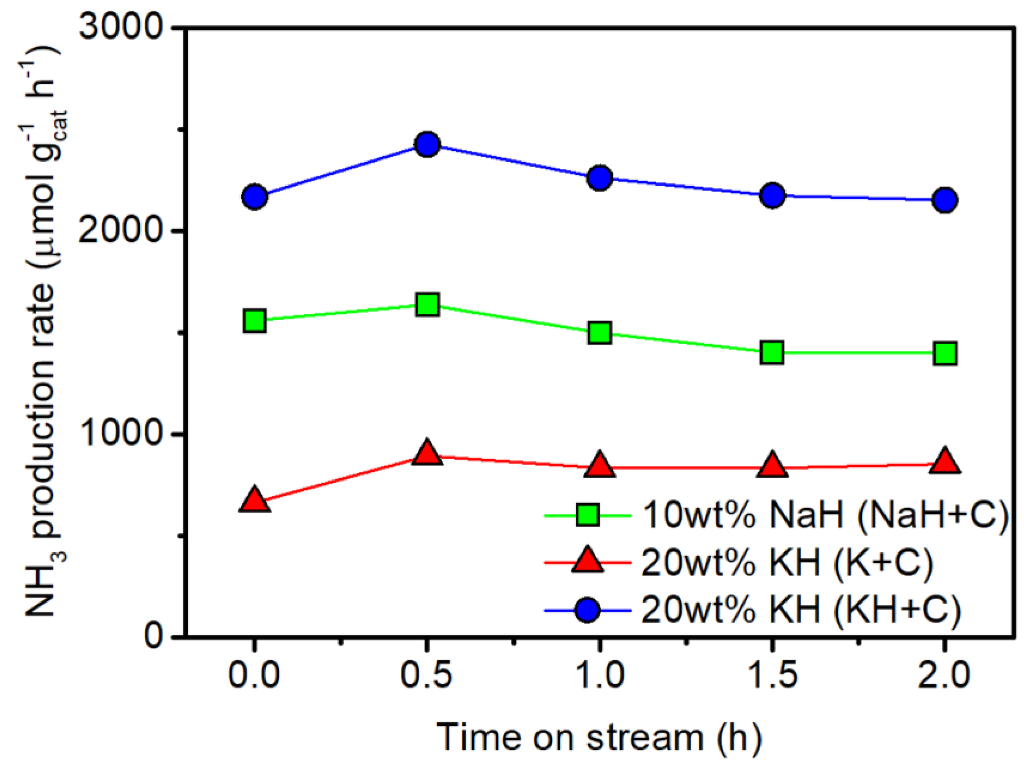


Reaction conditions NH_3 synthesis

- 10 bar, 300-400°C and 36,000 mL g_{cat}^{-1} h^{-1}
- Gas composition H_2:N_2 (molar ratio 3:1)

Catalyst stability: starting materials

Both the use of the hydride phase and the metallic phase lead to similar trends in initial activation and later slight deactivation at high temperature (400°C).



Key findings:

- AH_xC_y (A = Li, Na, K) nanocomposites were synthesized via melt infiltration and intercalation treatment.
- KH decomposition in the presence of microporous carbon leads to the formation of KH_xC_y.
- AH_xC_y (A = Li, Na, K) nanocomposites were found to be active towards ammonia synthesis.
- KH_xC_y nanocomposites were found to exhibit the best catalytic activity.

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References

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