

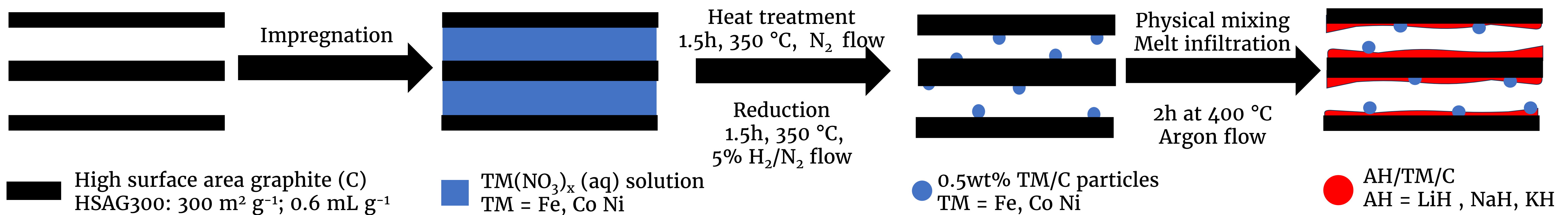
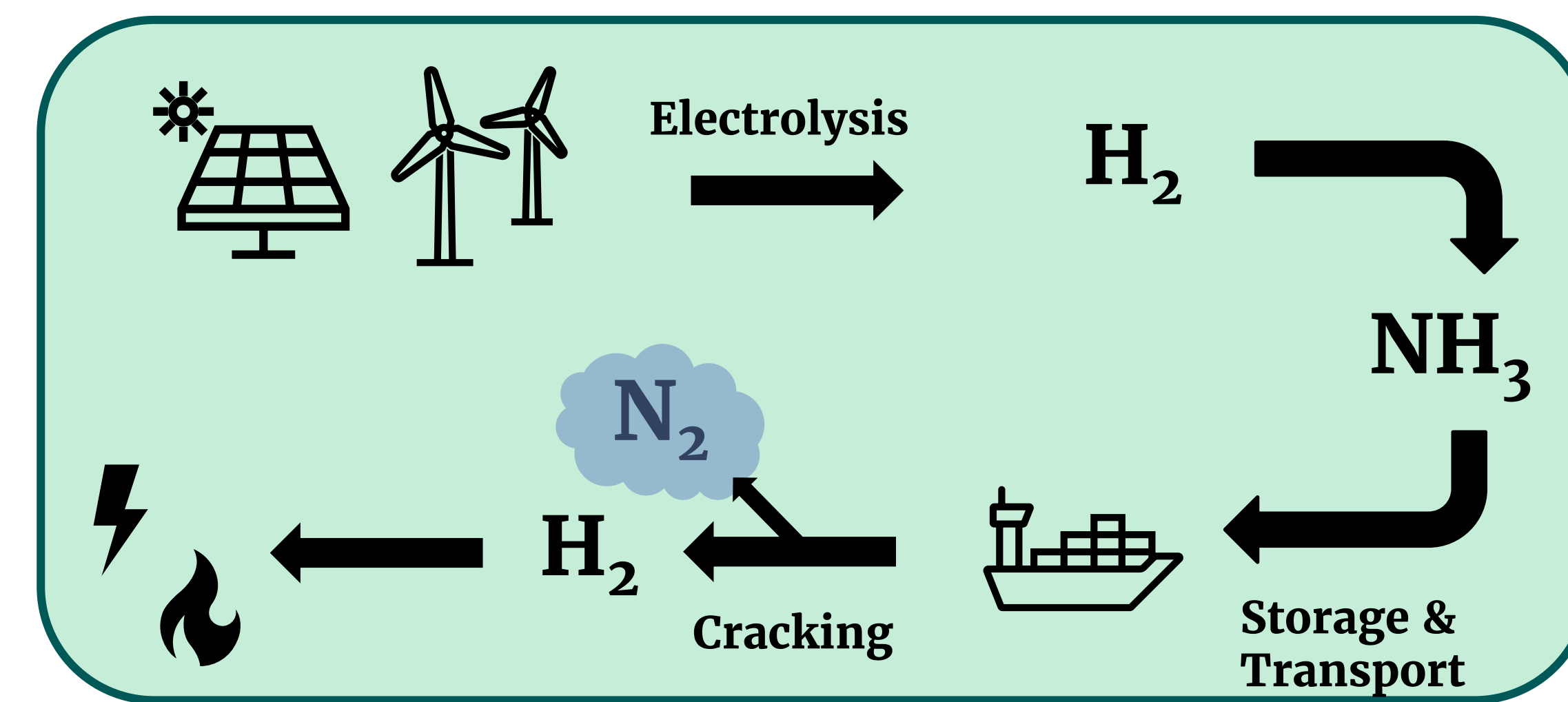
The key to efficient ammonia synthesis: The interplay between transition metal and alkali hydrides

Juliette C. Verschoor^{*1}, Pepijn Tils^{*}, Petra. E. de Jongh^{*}, Peter Ngene^{*}
^{*}Materials Chemistry and Catalysis, Utrecht University, The Netherlands
 j.c.verschoor@uu.nl

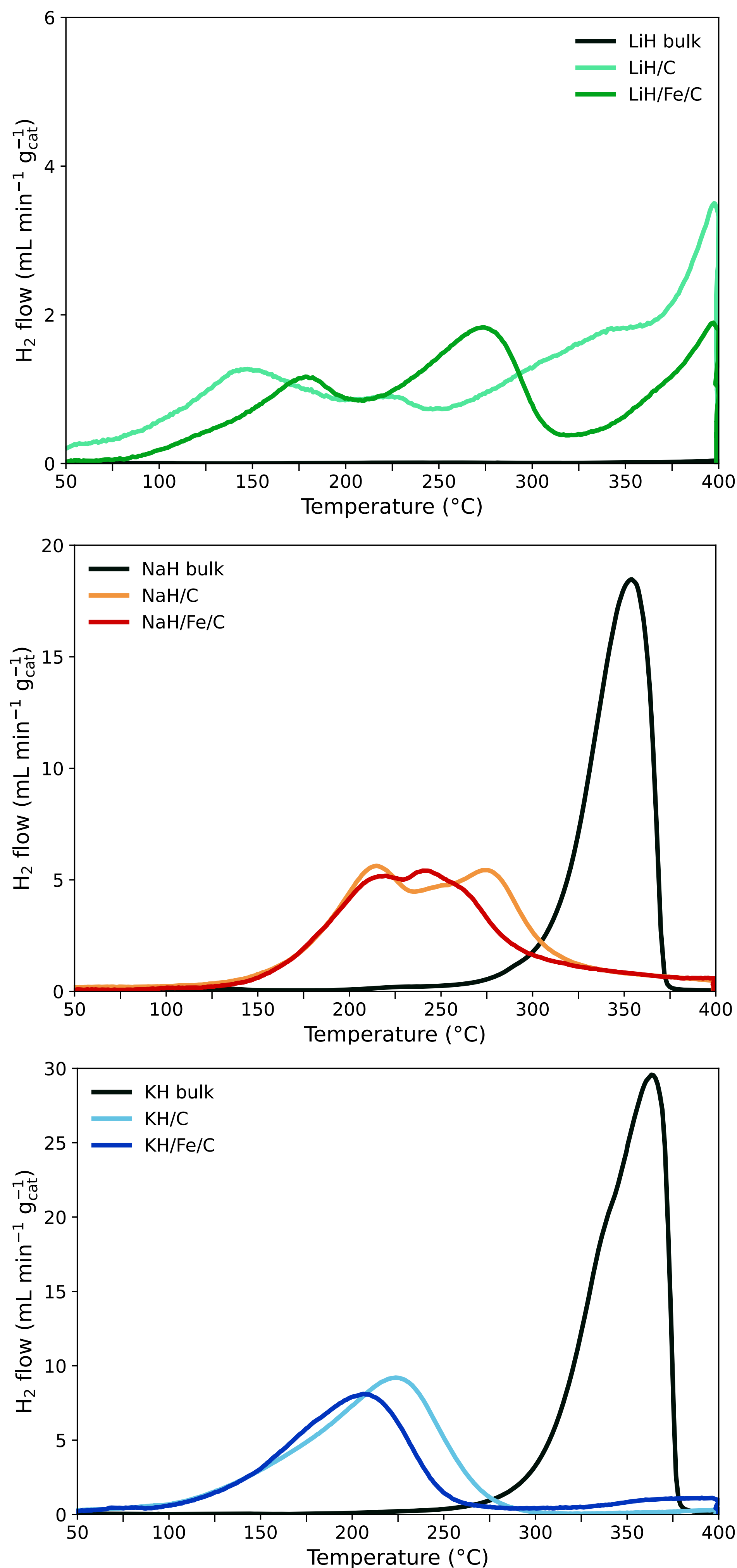
Ammonia (NH₃) is a crucial feedstock for fertilizer production and has recently gained attention as a promising hydrogen carrier for sustainable energy.¹ Yet, the strong nitrogen triple bond and scaling relations between adsorption and activation energies limit catalyst optimization. Consequently, industrial Fe- and Ru-based systems require harsh conditions (p > 100 bar, T > 450 °C), making catalysis under milder conditions difficult to achieve.

Here we demonstrate that nanoconfinement of alkali metal hydrides (AH = LiH, NaH, KH) together with a transition metal (TM = Fe, Co, or Ni) in graphitic carbon material (HSAG300) leads to high catalytic activity for ammonia synthesis at very moderate conditions (10 bar, 250–425 °C). This is due to nanoconfinement effects², which facilitate interaction between the transition metal and the hydride.³ The confinement and close contact with the graphitic carbon also destabilize the alkali hydrides, leading to N₂ and H₂ activation to NH₃ under these moderate conditions, even without the TMs. This cooperative effect opens up new routes toward more efficient and energy-saving ammonia synthesis.

Renewable energy to carbon-free fuels

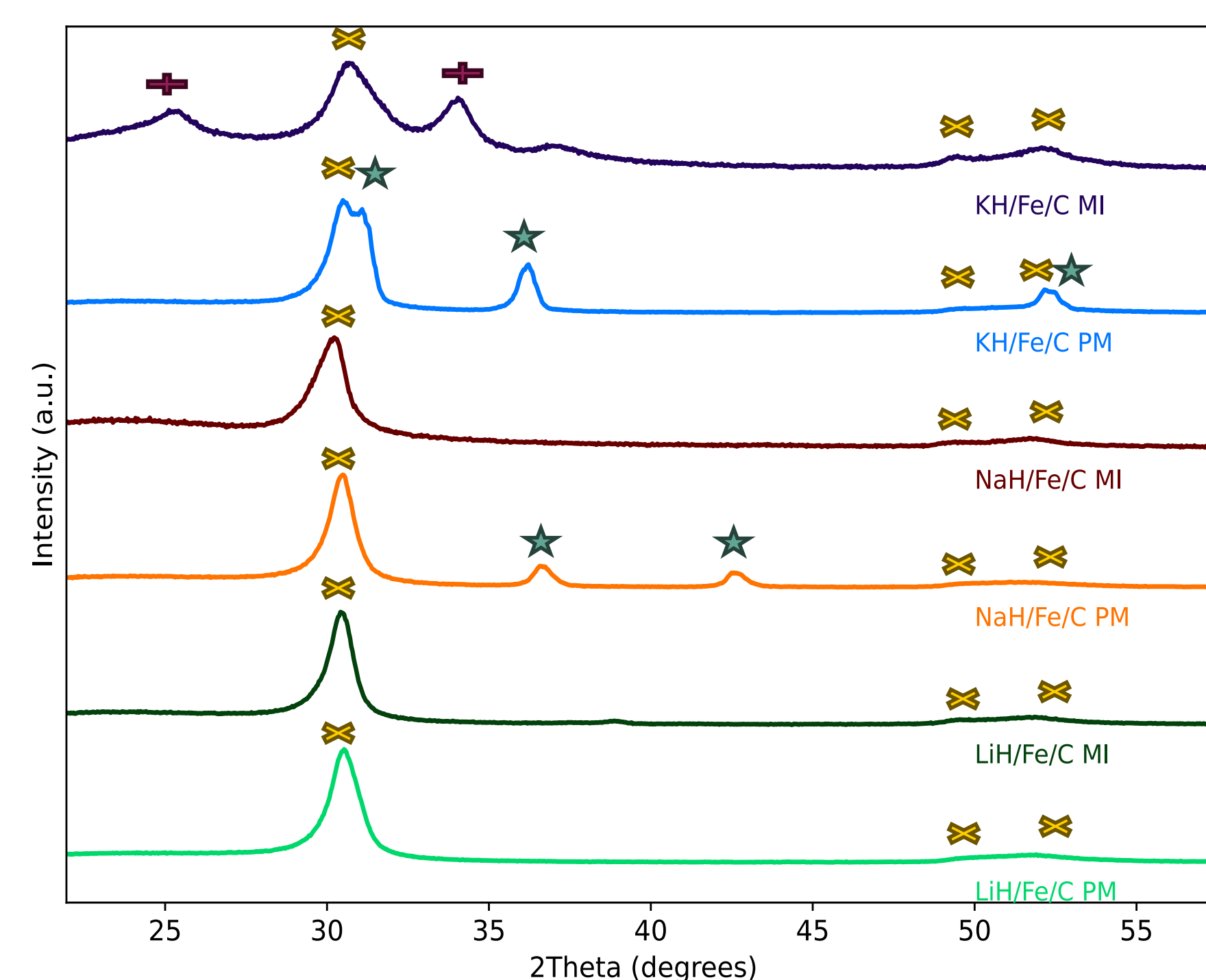


Alkali Hydride Decomposition



The presence of microporous carbon facilitates low-temperature AH decomposition

Crystallographic Phases



- ★ AH peaks disappear after melt infiltration
- ✚ KH intercalates into the carbon supports
- ✕ C remains largely unchanged

Key findings:

AH/TM/C nanocomposites were synthesized via melt infiltration

The presence of microporous carbon lowers the AH decomposition temperature and decreases crystallinity

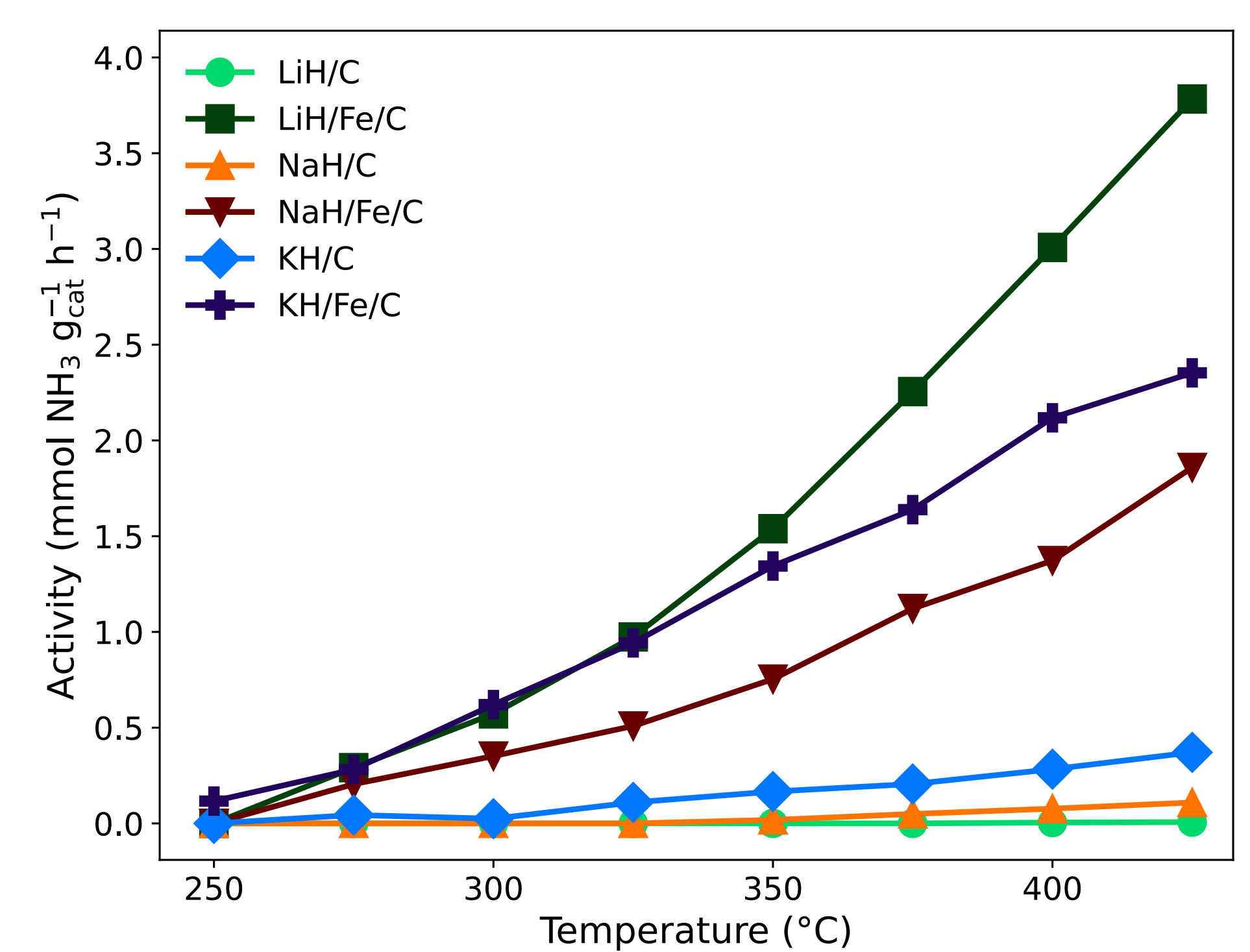
Melt infiltration of KH leads to the formation of intercalated KH_xC_y

AH/TM/C nanocomposites were active for ammonia synthesis

Acknowledgements:

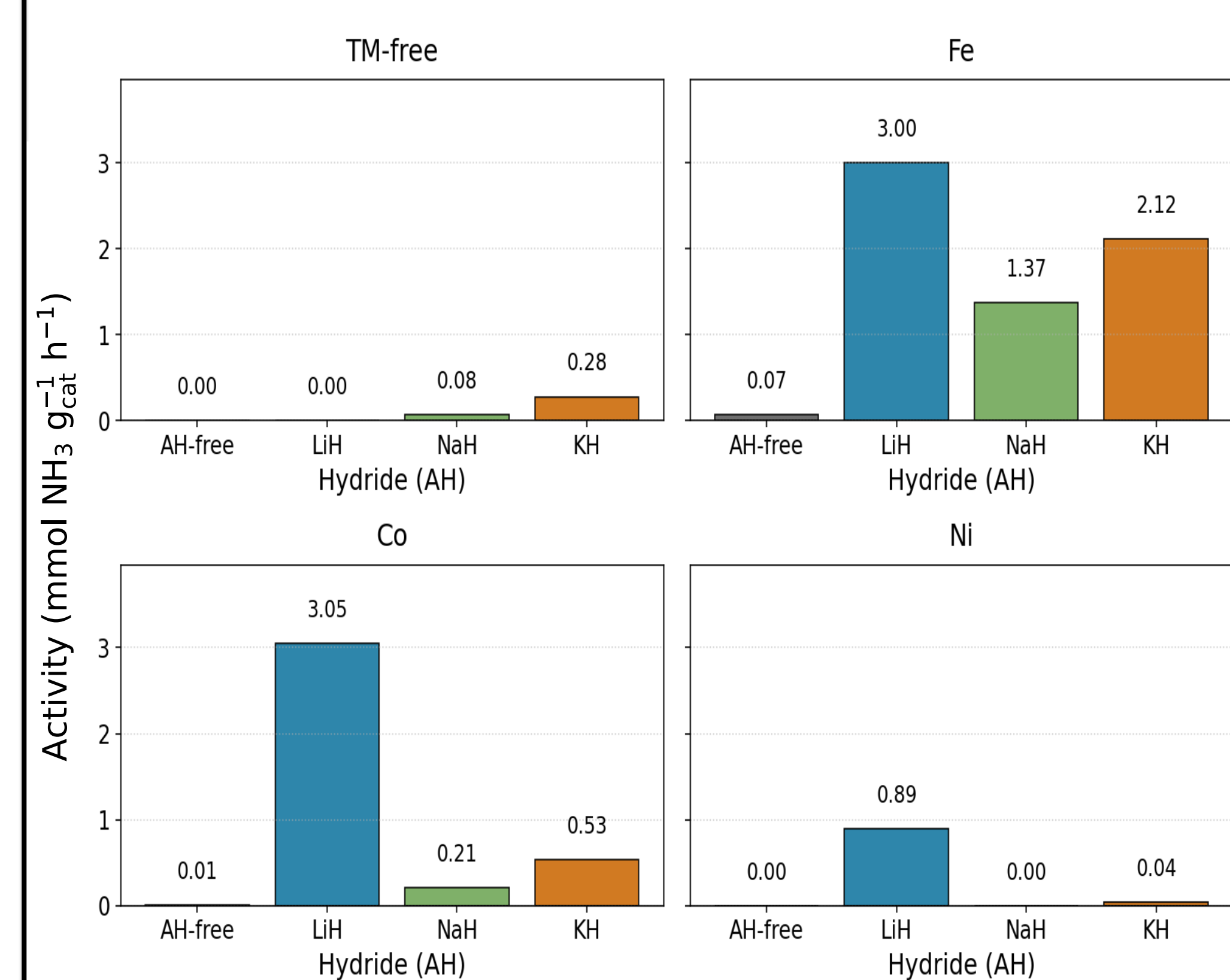
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Catalytic Activity: AH/Fe/C



AH/C nanocomposites are active for NH₃ synthesis
 The addition of Fe increases the catalytic activity significantly

Catalytic Activity: AH/TM/C



LiH/TM/C shows the highest activity for all TMs
 AH/Ni/C shows the lowest activity for all AHs

1. Guo, J., & Chen, P. (2017). Catalyst: NH₃ as an energy carrier. *Chem*, 3(5), 709-712.

2. Chang, F., et al. (2022). Potassium hydride-intercalated graphite as an efficient heterogeneous catalyst for ammonia synthesis. *Nature Catalysis*, 5(3), 222-230

3. Wang, Peikun, et al. "Breaking scaling relations to achieve low-temperature ammonia synthesis through LiH-mediated nitrogen transfer and hydrogenation." *Nature chemistry* 9.1 (2017): 64-70.

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