

# Catalyst Innovation to Enable Ammonia as A Hydrogen Carrier

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Background

Hydrogen (H<sub>2</sub>) is vital for decarbonisation, but its low volumetric density makes compression and transport prohibitively expensive. Ammonia (NH<sub>3</sub>) offers a viable hydrogen carrier, with 17.8 wt.% hydrogen, mild liquefaction conditions, and an existing shipping infrastructure that cuts transport costs by over 60% compared to liquid H<sub>2</sub>. However, adopting this supply chain requires efficient cracking technologies to release H<sub>2</sub> on demand.

$$\text{NH}_3 \rightarrow \text{H}_2 + \text{N}_2$$

Currently, ruthenium (Ru) catalysts operate below 500 °C but are constrained by high cost, scarcity, and deactivation (**Figure 1a**). Earth-abundant transition metals (Ni, Co, Fe) are cheaper but require temperatures above 600 °C due to sluggish N–H bond activation and N–N recombination, imposing heavy energy penalties. Cracking below the critical 500 °C threshold is essential not only to match Ru productivity benchmarks, but also to integrate directly with state-of-the-art solar-thermal reactors (**Figure 1b**). Developing active, noble-metal-free catalysts in this temperature window is key to enabling low-cost, zero-emission, solar-driven hydrogen production (**Figure 2**).

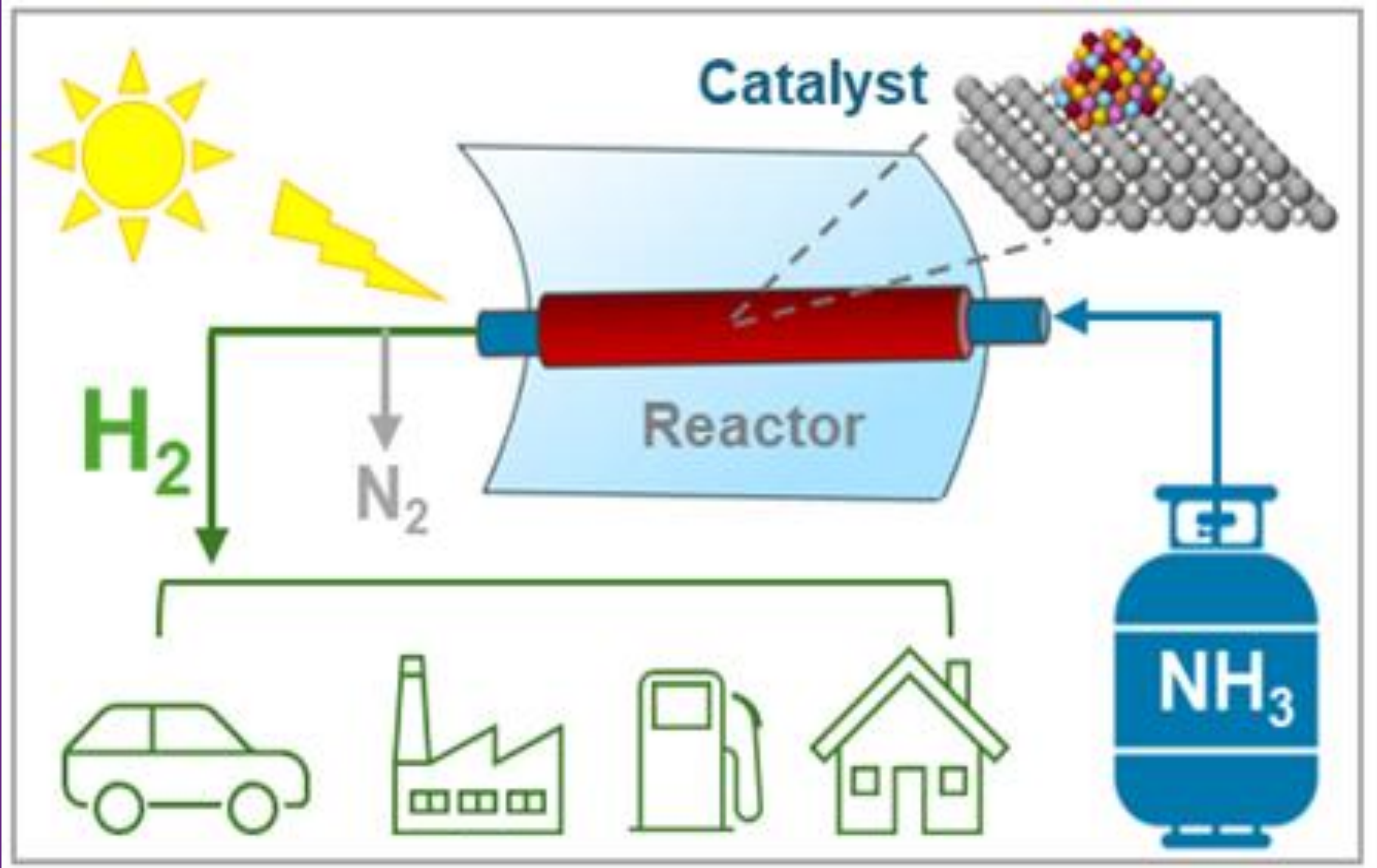


Figure 2. Solar-powered ammonia-to-hydrogen technology.

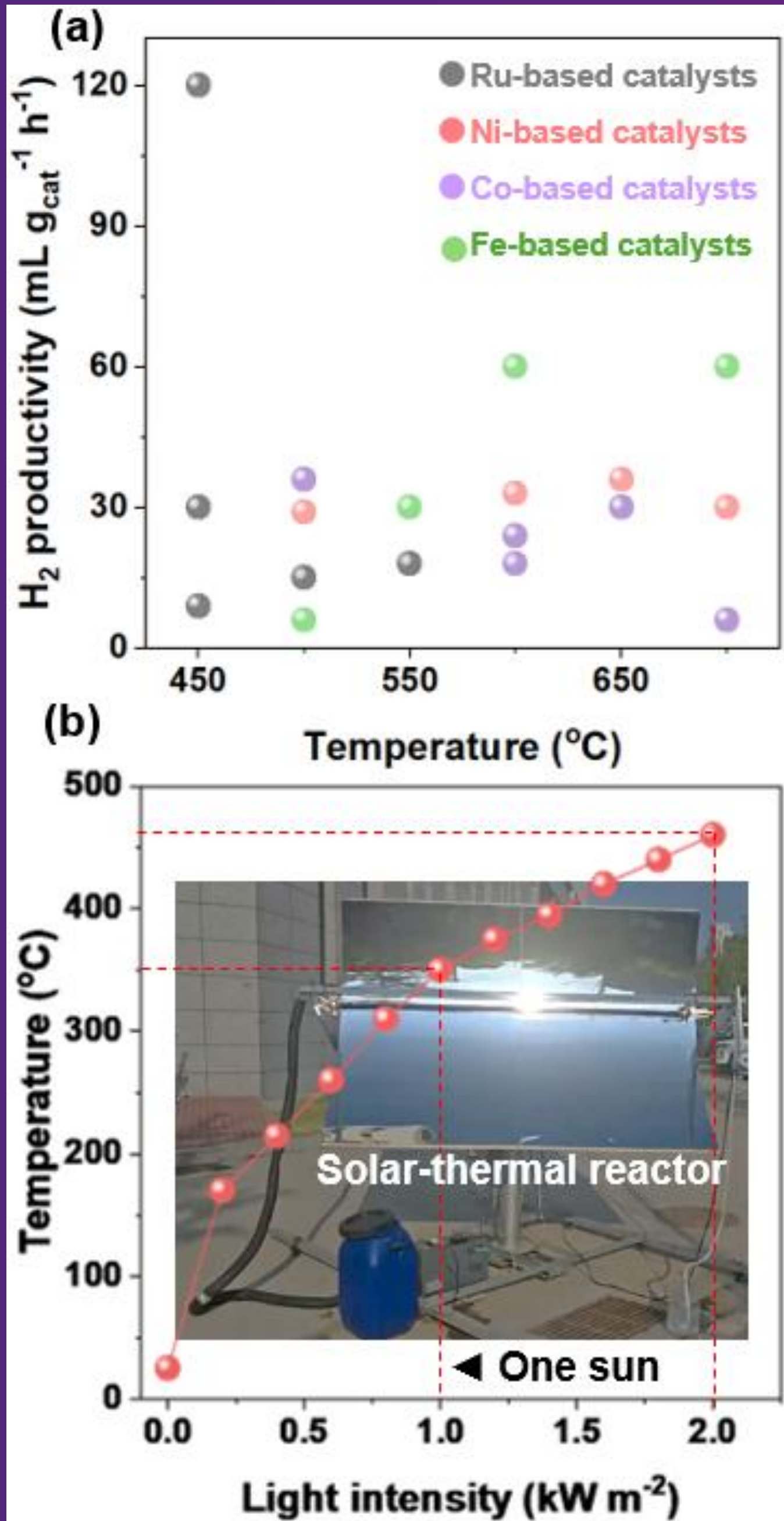


Figure 1. (a) H<sub>2</sub> productivity from ammonia decomposition on various metal-based catalysts. (b) The temperature of the solar-thermal reactor is related to the light intensity (1 kW m<sup>-2</sup> equals one sun)

Key Innovation

**ML-Accelerated Design of Low-Temperature Catalysts:** The first innovation is Machine Learning (ML)-guided discovery of noble-metal-free catalysts active below 500 °C. Currently, transition metals such as Ni or Fe require >600 °C, whereas only expensive noble metals operate in the desired sub-500 °C regime. We utilise ML to navigate the vast compositional space of high-entropy alloys (HEAs), identifying optimal solid-solution combinations that bypass traditional trial-and-error discovery. By predicting local electronic environments that lower the barriers to N–H bond cleavage and facilitate nitrogen recombination, ML identifies high-performance candidates for synthesis (**Figure 3**). This approach directly supports Objective 1 by delivering rational, cost-effective catalyst designs. Crucially, achieving activity at <500 °C aligns the chemistry with the capabilities of solar-thermal reactors, enabling a 100% renewable decomposition process that eliminates fossil-fuel dependence and carbon emissions.

**Machine learning-guided catalyst design**

- Electronegativity
- Lewis acidity
- d-bands filling
- Coordination number
- Neighbour atoms

**Activity**  
**Selectivity**  
**Stability**

**AI**

**High Entropy Alloys**

**Key steps: N-H breaking; N-N recombination; N<sub>2</sub> desorption**

Figure 3. Machine-learning-guided design of high-entropy alloys for ammonia decomposition.