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# Data-driven optimization of $NH_3$ decomposition catalysts

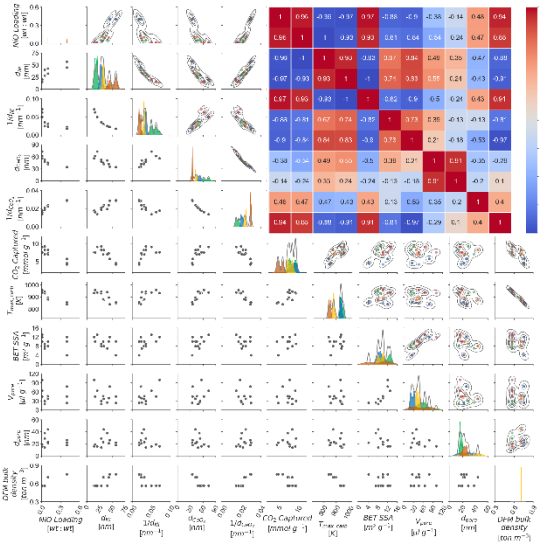
## Aim

The aim of this project is to make use of literature data for the design and synthesis of new high-performance $NH_3$ decomposition catalysts with consecutive testing.

## Justification

Ammonia is the second most produced chemical globally, with around 88% of its demand stemming from its critical role in fertilizer production. As the world shifts towards decarbonizing energy systems, ammonia decomposition emerges as a highly promising method for on-site, on-demand hydrogen generation. When produced using hydrogen with a very low carbon footprint, ammonia can serve as an efficient carrier and source of carbon-free hydrogen, further supporting the global energy transition towards cleaner and more sustainable solutions.

Advantages of ammonia include (i) its high volumetric and gravimetric hydrogen density[1], (ii) the relatively low minimum energy penalty of 16% required for its decomposition[2], and (iii) the very low levels of contaminants in the hydrogen product[3] compared to methane/methanol-reforming, reducing the energetic and economic burden of downstream separation.



*Example of correlation analysis for the investigation of Synthesis-Property-Performance relationships.*

## Program

- Literature survey to establish a database for synthesis-property-performance correlation analyses of $NH_3$ decomposition catalysts.
- Correlation analyses and identification of the main drivers for catalyst performance using data science packages available for Python.
- Formulation of next-generation $NH_3$ decomposition catalysts based on correlation analyses.
- Synthesis, characterization and testing of next-generation $NH_3$ decomposition catalysts.

## References

(1) Mukherjee, S.; Devaguptapu, S. V.; Sviripa, A.; Lund, C. R. F.; Wu, G. Low-temperature ammonia decomposition catalysts for hydrogen generation. *Applied Catalysis B: Environmental* **2018**, *226*, 162-181. DOI: https://doi.org/10.1016/j.apcatb.2017.12.039.

(2) T-Raissi, A. *Technoeconomic Analysis of Area II, Hydrogen Production Part II: Hydrogen From Ammonia and Ammonia-Borane Complex for Fuel Cell Applications,"* 2002.

(3) Lipman, T.; Shah, N. Ammonia as an Alternative Energy Storage Medium for Hydrogen Fuel Cells: Scientific and Technical Review for Near-Term Stationary Power Demonstration Projects, Final Report. *Institute of Transportation Studies, UC Berkeley, Institute of Transportation Studies, Research Reports, Working Papers, Proceedings* **2007**.

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