

## Ab Initio Multiscale Catalytic Synthesis/Cracking Reaction Modelling of Ammonia as Liquid Hydrogen Carrier

**Authors :** Blaž Likožar, Andraž Pavlišič, Matic Pavlin, Taja Žibert, Aleksandra Zamljen, Sašo Gyergyek, Matej Huš

**Abstract :** Ammonia is gaining recognition as a carbon-free fuel for energy-intensive applications, particularly transportation, industry, and power generation. Due to its physical properties, high energy density of 3 kWh kg<sup>-1</sup>, and high gravimetric hydrogen capacity of 17.6 wt%, ammonia is an efficient energy vector for green hydrogen, capable of mitigating hydrogen's storage, distribution, and infrastructure deployment limitations. Chemical storage in the form of ammonia provides an efficient and affordable solution for energy storage, which is currently a critical step in overcoming the intermittency of abundant renewable energy sources with minimal or no environmental impact. Experiments were carried out to validate the modelling in a packed bed reactor, which proved to be agreeing.

**Keywords :** hydrogen, ammonia, catalysis, modelling, kinetics

**Conference Title :** ICCBE 2024 : International Conference on Chemical and Biochemical Engineering

**Conference Location :** Zurich, Switzerland

**Conference Dates :** July 29-30, 2024