

Ammonia synthesis by chemical looping via hydrolysis of binary nitrides

Enkhtsetseg Dashjav, Daniel Koch, Lena Klaas, Mathias Pein, Martin Roeb

Institute of Future Fuels, German Aerospace Centre (DLR), Cologne, 51147, Germany,

Keywords: chemical looping synthesis of ammonia, green ammonia fertilizer, redox cycling of nitrides and oxides

Ammonia and its sustainable production are increasingly becoming the focus of current research. The production of green ammonia—utilizing integrated solar thermal energy—is part of our research at the Institute of Future Fuels of the German Aerospace Center.

Klaas et al. have reviewed four mild-condition ammonia production methods and demonstrated that chemical looping is a promising alternative to the Haber-Bosch process, which requires high amounts of fossil energy¹. To date, there is a lack of systematic studies on ammonia looping synthesis. Therefore, we have initiated a systematic theoretical and experimental study on ammonia synthesis via redox cycling of binary metal oxides and nitrides, using H₂O as a hydrogen source. These activities will be accompanied by a process and techno-economic analysis to evaluate the feasibility of a pilot production line.

This concept has already been experimentally demonstrated by the Abanades group and others^{2, 3}. Within this work, recent results from ab-initio calculations such as DFT are presented and evaluated alongside available data from literature. Valuable insights into reaction conditions, kinetics, and overall feasibility are provided and discussed.

1. Klaas, L.; Guban, D.; Roeb, M.; Sattler, Ch.(2021): *International Journal of Hydrogen Energy* 46 (49), S. 25121–25136. DOI: 10.1016/j.ijhydene.2021.05.063.

2. Abanades, S; Rebiere, B.; Drobek, M.; Julbe, A. (2024): *Chemical Engineering Science* 283, S. 119406. DOI: 10.1016/j.ces.2023.119406.

3. Gao, X; Bush, H. Evan; Miller, J.; Bayon, A.; Ermanoski, I.; Ambrosini, A.; Stechel, E.B. (2023): *Chemistry of Materials* 35 (15), S. 5864–5875. DOI: 10.1021/acs.chemmater.3c00606.