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Solar-driven thermochemical production of ammonia via a metal nitride cycle

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1. Motivation

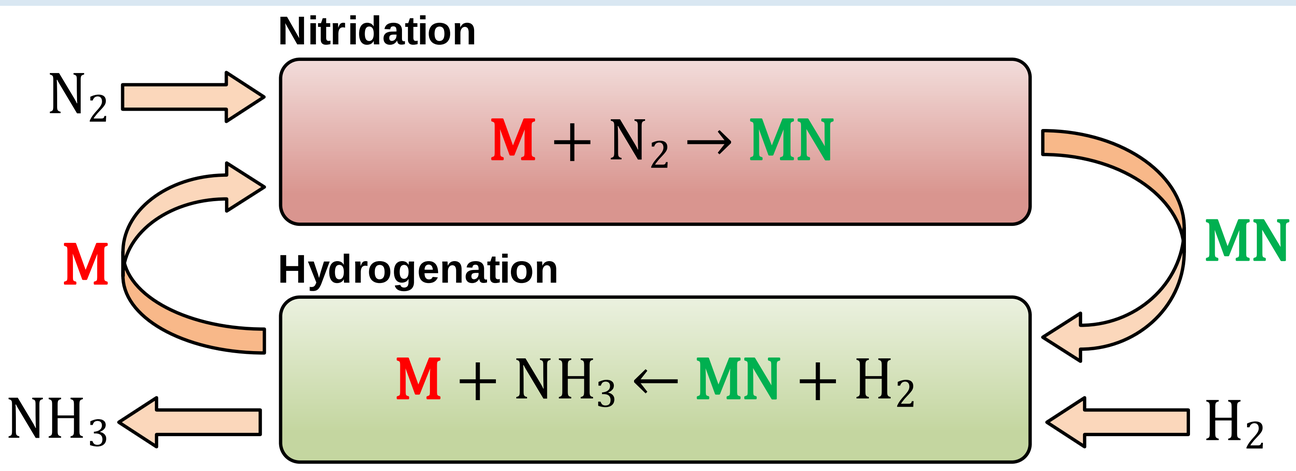
Solar Thermochemical Ammonia

- Reduced CO_2 emissions compared to Haber-Bosch
- Low pressures (1-60 bar)
- Cheaper, decentralized production plants

2. Solar Thermochemical Ammonia Production

Reaction

- Two-step thermochemical cycle
- Hydrogenation: low temperature (100-200 °C) reaction of metal nitride **MN** with H_2
- Nitridation: high temperature (500-1000 °C) reaction of pure metal **M** with N_2



3. Methods & Results

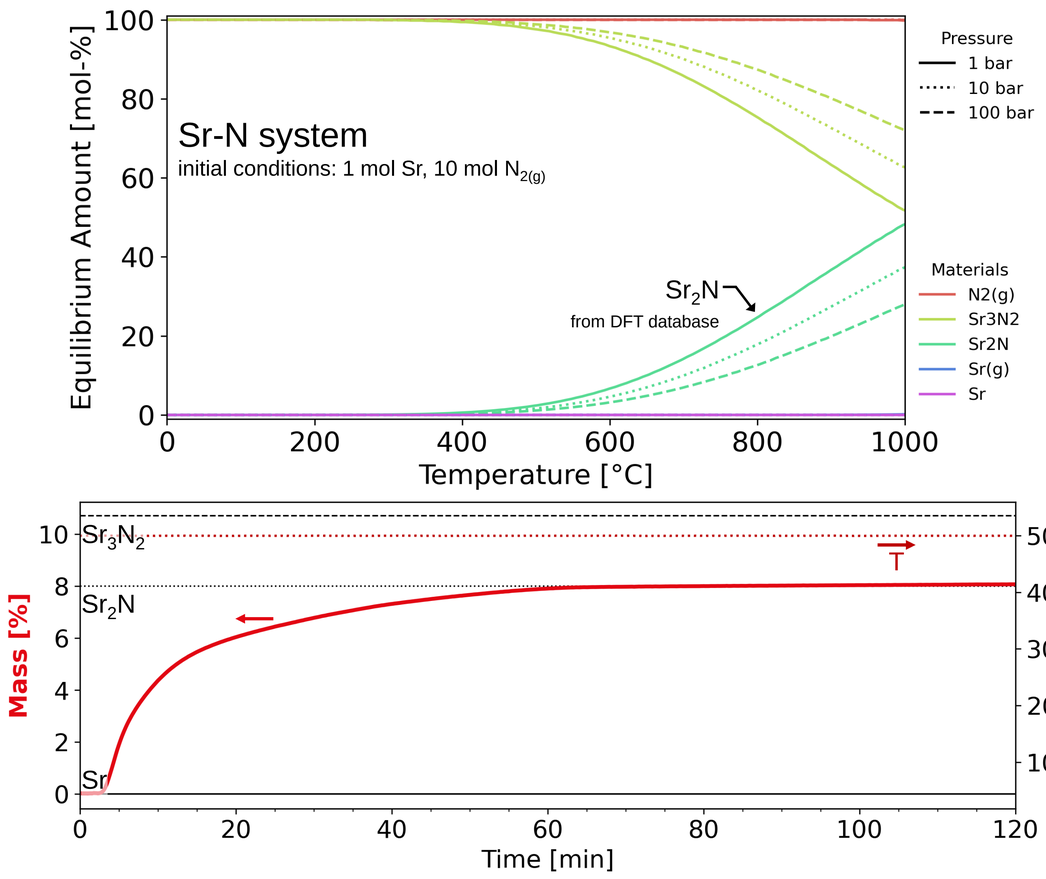
Computational Screening

- Theoretical data from DFT database
- Equilibrium plots to estimate species

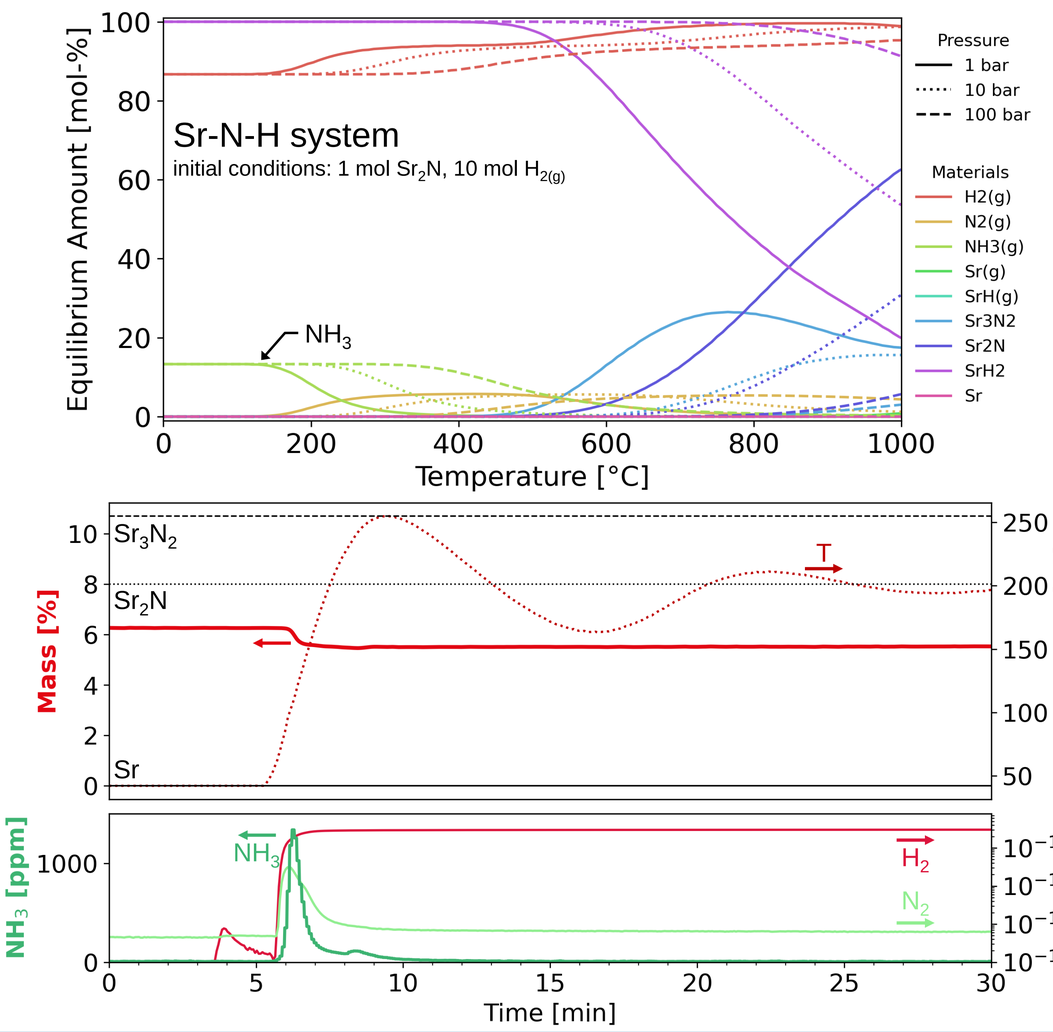
Experimental Validation

- Performance assessment with TGA
- Mass balance with gas analysis

1st step: Nitridation of Sr



2nd step: Hydrogenation of Sr_2N



4. Key Messages

- 11 binary, 6 ternary metal nitrides screened: Sr, Ca, Cr, Mn, Fe, Co, Ni, Cu, Zn, Mo, W
- Sr identified as best performing material
- Demonstrated first quantitative measurement of ammonia