SAND2020-2337C

PROJECT NAME: Solar Thermochemical Ammonia Production (STAP)

Last 5 digits of project number: **34250**

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BACKGROUND / INDUSTRY IMPACT

- Ammonia (NH_3) is a vital component of fertilizer and other commodity chemicals
- Current production (Haber-Bosch) requires high T and P, and accounts for >1% of world CO_2 emissions
- Development of renewable, low-carbon NH_3 can enable production of fertilizer and chemicals with greatly decreased carbon footprint.

PROJECT OVERVIEW / OBJECTIVES

- Objective: Develop a solar thermochemical looping technology to produce and store N_2 from air for the subsequent production of NH_3 via an advanced two-stage process
- The novelty of the process is the development of metal nitride (MN) materials that will produce NH_3 via a cyclic solid-state reduction reaction with H_2

METHODS

- Synthesize metal oxide and metal nitride materials for N_2 recovery NH_3 synthesis, respectively
- Model/design/construct/demonstrate lab-scale reactors for solar receiver, N_2 separation, and NH_3 production
- Develop technoeconomic models to estimate costs, sensitivities, efficiency, and integration with CST and identify a path toward scale-up and commercialization

KEY OUTCOMES / MILESTONES

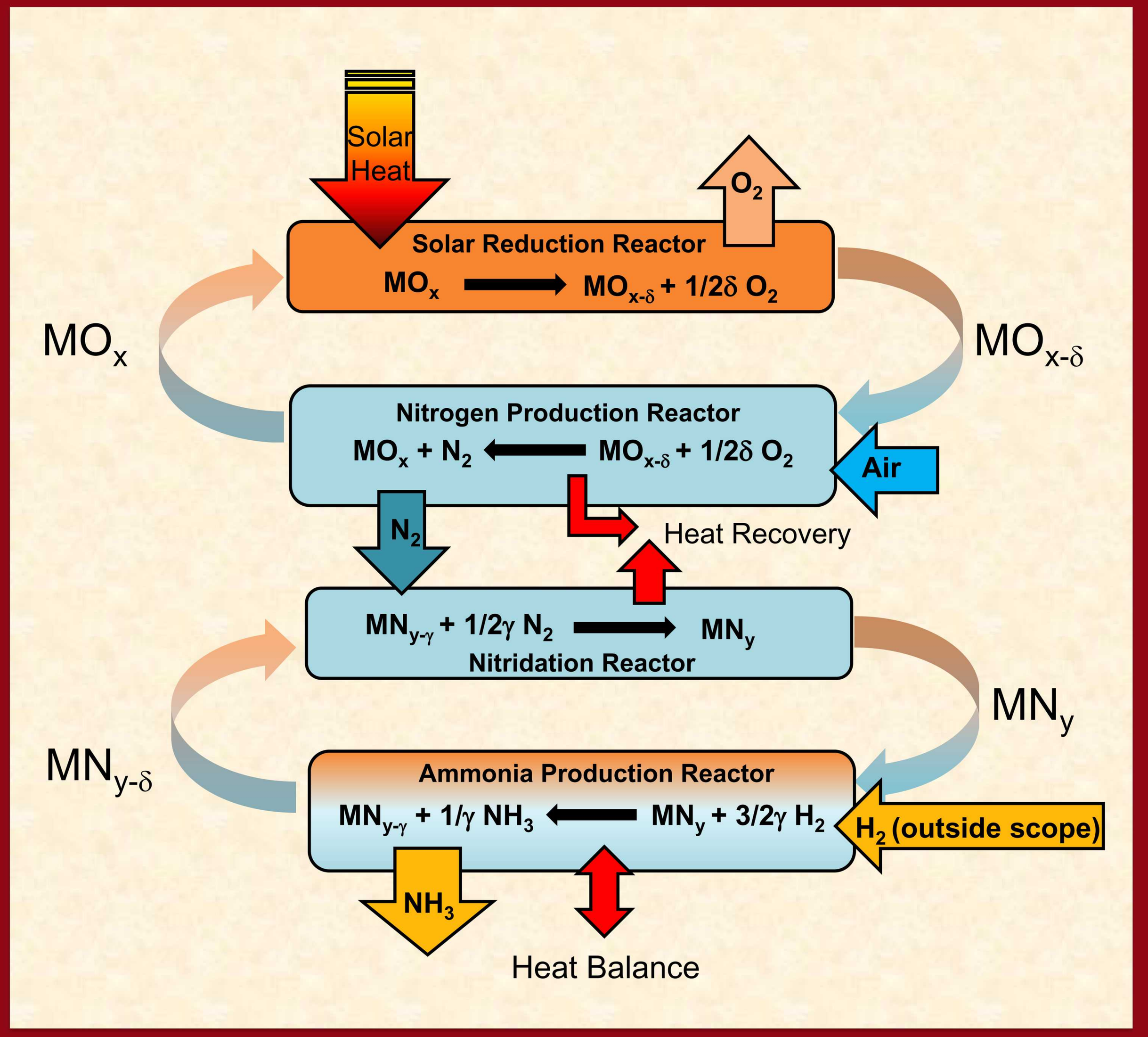
- Ba- and La-doped $SrFeO_3$ were synthesized, characterized, and selected as oxide materials for N_2 separation from air based on redox performance and economics
- Several ternary nitride compounds were identified as potential materials for NH_3 synthesis
- SIERRA/Aria functionalities were developed to capture the primary physics of multiphase transport, heat transfer, and chemical reactivity within oxide reactor models
- System models developed for Haber-Bosch and N_2 separation processes.

CONCLUSION / REMAINING RISK

- Successful completion of this project will result in a demonstration of a novel route to NH_3 production via a renewable, carbon-free technology with a path to scale-up and integration with a CSP plant.
- Development of metal oxide system for separation of N_2 is on track. Materials have been identified and reactor modeling proceeds apace.
- Systems modeling and technoeconomic analysis informing and complimenting reactor development
- Major Risk: Synthesis of ternary nitride material has proven challenging and put the nitride effort behind schedule. Alternate syntheses under consideration.

CONCENTRATING SOLAR-THERMAL POWER TRACK (High-Temperature Thermal Systems)

Renewable, CO_2-free ammonia production technology with a path to scale-up integration with CSP



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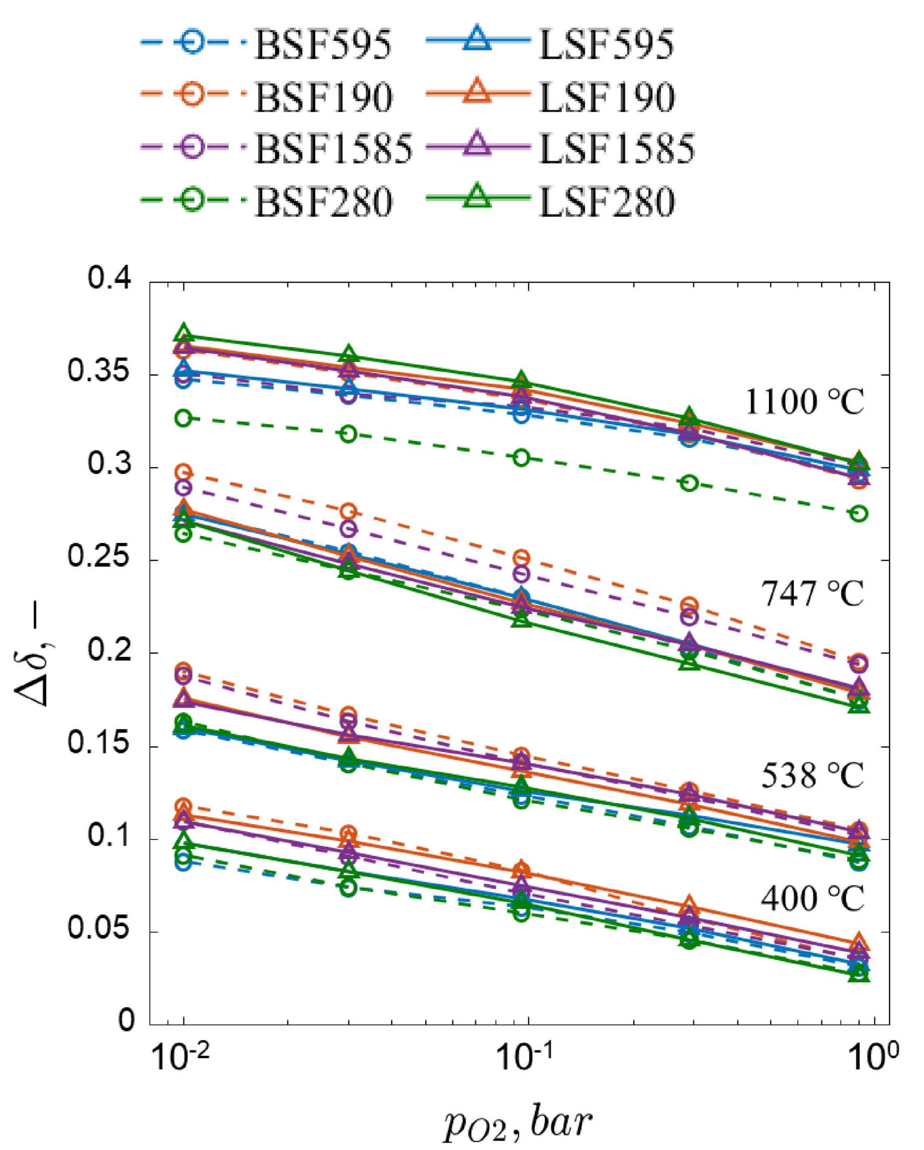
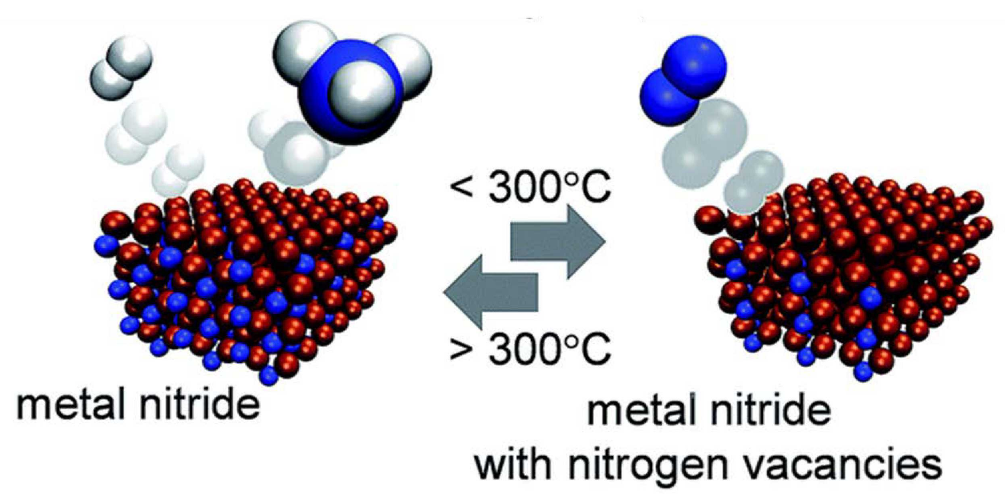
Co-PIs: Peter Loutzenhiser (GIT), Ellen Stechel (ASU), Ivan Ermanoski (ASU), Kevin Albrecht (SNL)

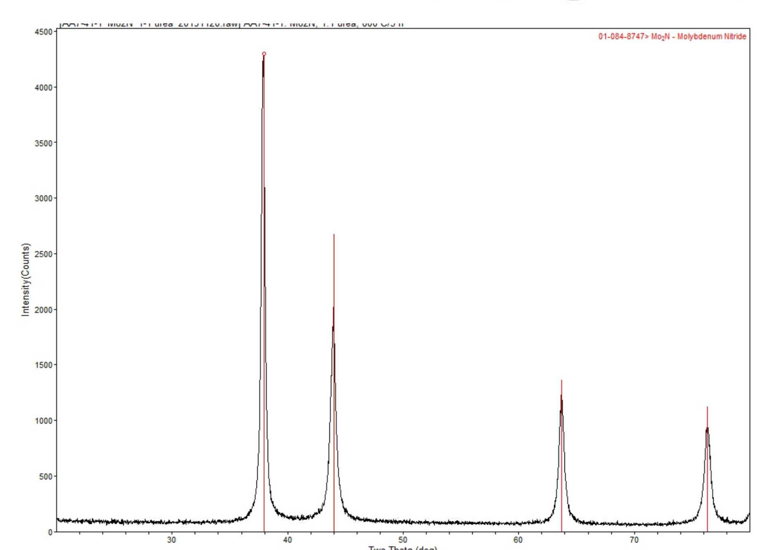


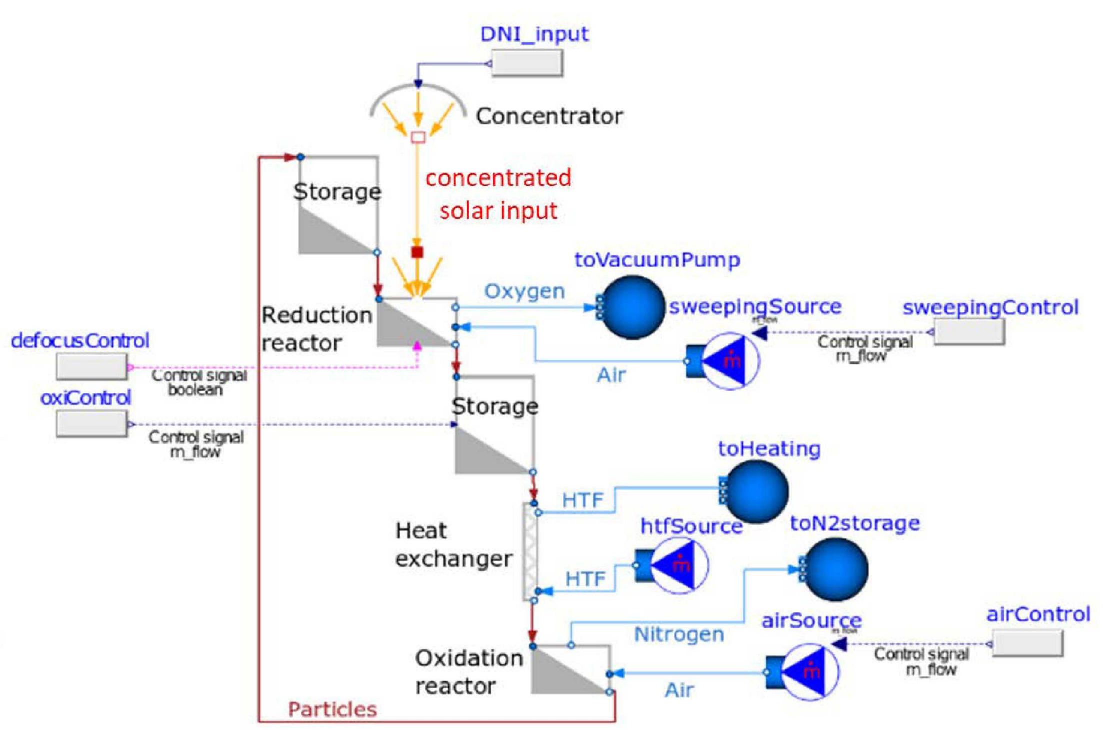
$Ba_xSr_{1-x}FeO_{3-\delta}$ and $La_xSr_{1-x}FeO_{3-\delta}$ nonstoichiometry (x= 0.05, 0.1, 0.15, 0.2) as a function of O_2 partial pressure and temperature.

Top: Representation of reversible ammonia formation via hydrogen reduction (left) and re-ntridation (right). Blue = N, red = M, white = H. (*from Michalsky, R., et al, Chem Sci, 6(7), 3965, doi: 10.1039/c5sc00789e*)

Bottom: X-ray diffraction pattern of Mo_2N synthesized via urea glass method.

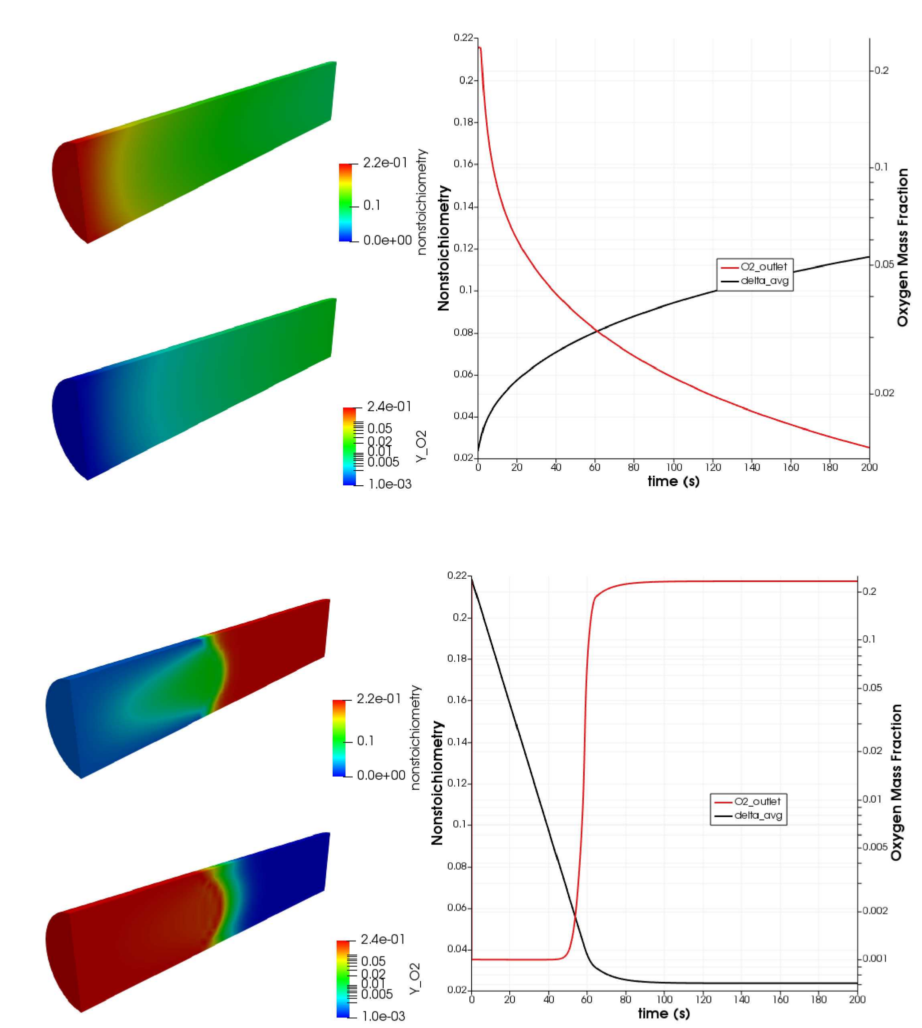






To calculate the annual amount of N_2 produced from STAP under solar conditions, a system model of the N_2 separation process has been developed. The model was implemented using Modelica. (www.modelica.org/documents)

Packed-bed reactor simulation of cyclic metal oxide using Aria porous media model to simulate solid-gas reacting system at 1000 °C.
(Top) Reduction using sweep gas with an oxygen partial pressure of 10^{-3} atm.
(Bottom) Oxidation using ambient air with an oxygen partial pressure of 0.21 atm.



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