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## Methanation Catalysts for Novel Sorption-Regeneration & Methanation Process

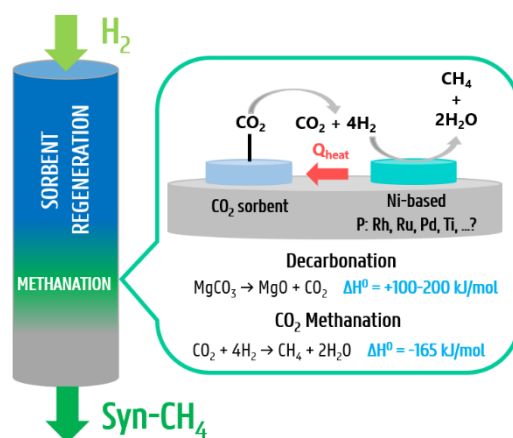
### Aim

- Develop highly-active and selective methanation catalysts for low-temperature CO<sub>2</sub> methanation for a novel integrated CCU process.
- Study methanation kinetics under low CO<sub>2</sub> partial pressures and various CO<sub>2</sub>/H<sub>2</sub> ratio's.

### Justification

The European Green Deal outlines steps to become the first continent to reach climate neutrality by 2050. In the wake of this climate crisis, Belgium faces a challenging transition to a sustainable, affordable and secure energy system. The large injection of intermittent renewable energy sources (RES) raises concerns about the security of energy supply and grid stability. In the future energy system, the conversion of electrical power to energy molecules will be crucial to eliminate these concerns. One of the conversion pathways looks at electrolytic (green) H<sub>2</sub>, which is associated with high transport and storage costs. Pathways to convert H<sub>2</sub> to synthetic methane are therefore becoming increasingly important in Belgium, given Belgium's large existing natural gas transport and storage infrastructure. This pathway, commonly known as the Sabatier reaction, uses H<sub>2</sub> to convert CO<sub>2</sub> to synthetic methane and heat losses (165 kJ/mol).

To acquire a suitable CO<sub>2</sub> stream for methanation, new capture technologies are needed to separate and isolate CO<sub>2</sub> from dilute CO<sub>2</sub> streams (< 10 mol% CO<sub>2</sub>). The high energy penalty (100-200 kJ/mol) of sorption using solid CO<sub>2</sub> adsorbents is associated with heating and regenerating the solid sorbent bed [1]. By coupling exothermic CO<sub>2</sub> methanation to endothermic desorption of CO<sub>2</sub> in an integrated CCU process, both the **reaction energy** and the **thermodynamic driving force** to regenerate the CO<sub>2</sub> sorbent are provided. To limit the energy penalty, a mild regeneration-methanation temperature is needed (<350°C). In this temperature region, novel Ni-based methanation catalysts display an excellent activity, selectivity and stability for stoichiometric reaction conditions [2, 3]. Depending on the sorbent performance, CO<sub>2</sub> release is expected to be slow and unusual CO<sub>2</sub>/H<sub>2</sub> ratio's can occur in the packed bed. The methanation kinetics at low CO<sub>2</sub> partial pressures must be further investigated with newly synthesized catalysts. In the final stage, the student will perform a quantitative analysis of the integrated capture-regeneration & methanation process. An existing proof-of-concept for "integrated capture-regeneration & methanation" already exists [4], but further quantification of the process using the optimized methanation catalyst is needed.



**Figure 1:** CO<sub>2</sub> methanation (carbonate reduction) using a supported Ni catalyst in an integrated CCU process.

### Program

1. Literature review: CO<sub>2</sub> methanation catalysts (role of support, promoters, kinetics)
2. Synthesis & characterization: (Ni-based) methanation catalysts with/without promoters
  - N<sub>2</sub> physisorption, TPR, TPD, XRD, STEM/HR-TEM, FTIR-DRIFTS, ...
3. Screening: evaluate the performance (activity/selectivity/stability) of newly synthesized methanation catalysts at mild temperatures, low CO<sub>2</sub> partial pressures, high/low CO<sub>2</sub>:H<sub>2</sub> ratio's
4. Optional: execute experiments generated by simulated testing conditions (see other thesis topic: **Dynamic Simulations of a Novel CCU Process Through Temperature-Swing Chemical Looping**)
5. Testing of CCU: quantify the performance of the integrated capture-regeneration & methanation process using a solid CO<sub>2</sub> sorbent and synthesized methanation catalyst.

## References

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2. Abelló, S., Berrueto, C., Gispert-Guirado, F., & Montané, D. (2016). Synthetic natural gas by direct CO<sub>2</sub> hydrogenation on activated takovites: effect of Ni/Al molar ratio. *Catalysis Science & Technology*, 6(7), 2305-2317. <https://doi.org/10.1039/c5cy01200g>
3. Shen, L., Xu, J., Zhu, M., & Han, Y.-F. (2020). Essential Role of the Support for Nickel-Based CO<sub>2</sub> Methanation Catalysts. *ACS Catalysis*, 10(24), 14581-14591. <https://doi.org/10.1021/acscatal.0c03471>
4. Mesters, C., Rahimi, N., van der Sloot, D., Rhyne, J., & Cassiola, F. (2021). Direct Reduction of Magnesium Carbonate to Methane. *ACS Sustainable Chemistry & Engineering*, 9(33), 10977-10989. <https://doi.org/10.1021/acssuschemeng.1c01439>