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Coach	**Supervisor(s)**	**Funding**
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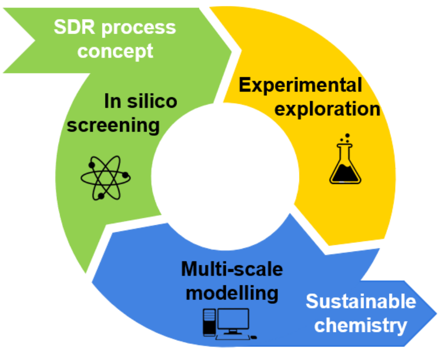
A combined computational and experimental study on super-dry reforming of methane for CO_2 conversion

Aim

This thesis aims at developing a multi-scale modelling approach for super-dry reforming and the optimisation of the materials used in this process.

Justification

Energy-intensive industries face the enormous challenge of reducing their greenhouse gas emissions and even closing the carbon cycle by converting CO_2 into valuable products, while keeping their activities competitive. Super-dry reforming of methane is a strongly intensified CO_2 conversion process as it converts up to 3 CO_2 molecules per molecule of CH_4 into a pure CO stream, which is an important building block for the chemical industry as well as an essential feedstock for the steel industry [1].



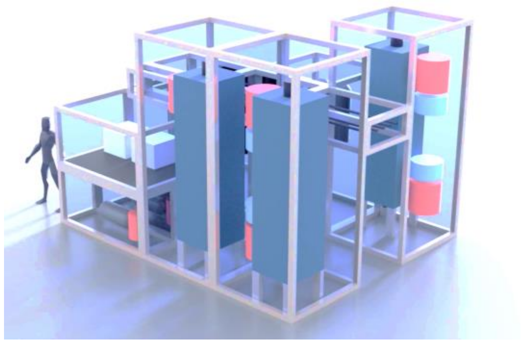


Figure 1. Super-dry reforming as a process concept for a more sustainable industry (*left*). The pilot unit which brings large-scale implementation of the process one step closer (*right*).

This cutting-edge technology was invented and developed at the LCT [2]. In September 2022, the very first super-dry reforming unit at pilot level (1 kg CO_2/h) will be built and commissioned (see Figure 1).

Program

- Literature survey on in silico screening of materials for the super-dry reforming process [3].
- Construction of a database with thermodynamic and kinetic parameters for chemical reactions involving nanoparticles obtained from high-level density functional theory calculations [4].
- Synthesis of nanomaterials for validation of quantum chemistry data.
- Perform experiments on the pilot unit to explore the effect of different bed configurations and for validation of an existing one-dimensional reactor model.

References

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