LABORATORY FOR CHEMICAL TECHNOLOGY
Technologiepark 125, 9052 Gent, Belgium

Coach	Supervisor(s)	Funding
Tong Liu Lukas Buelens	Kevin Van Geem Vladimir Galvita	

High-Throughput Catalyst Screening for Chemical Looping Dry Reforming of Methane Using Machine Learning and DFT Methods

Aim

The research aims to develop an efficient screening method of materials through high-throughput to get high-activity catalysts for chemical looping dry reforming of methane.

Justification

Chemical looping dry reforming of methane is a technology that couples the selective oxidation of methane with the cyclic reduction of carbon dioxide, enabling the efficient conversion and utilization of two major greenhouse gases. This process critically depends on high-performance catalysts. However, the current catalyst screening primarily relies on experimental trial-and-error methods, which are time-consuming and inefficient. The integration of machine learning (ML) and density functional theory (DFT) represents an emerging and transformative paradigm for the design and screening of high-performance materials. DFT enables the prediction of physicochemical properties of materials, thereby reducing the need for repetitive experimental synthesis and testing. Nonetheless, relying exclusively on DFT calculations can be computationally intensive and time-consuming. ML offers a solution by accelerating the high-throughput screening process, leveraging its ability to map the relationship between material structural features and energy properties. This research seeks to combine ML and DFT to establish an innovative framework for catalyst development, offering valuable insights and practical guidance for the discovery and optimization of high-activity materials.

Program

- DFT calculations will be performed to determine properties such as formation energy, Gibbs free energy, and oxygen vacancy formation energy, validating the positive correlation between energy characteristics and catalytic reactivity.
- Based on the DFT results, a database of catalyst characteristics and energy descriptors will be established.
- Several different models will be evaluated and a highly accurate model will be selected to predict the performance of a large number of catalysts.
- A selection of catalysts with good overall performance will be selected and synthesized for those catalysts, reactivity and cyclic stability tests for chemical looping dry reforming of methane will be conducted to obtain the best catalyst.