**CO2 capture and separation using metal-organic frameworks: effect of amine-functionalization and framework flexibility**

By Sarah Couck
Department of Chemical Engineering (CHIS)
Advisor: Prof. Joeri Denayer

Reducing the $CO_2$ levels in the atmosphere is one of the emerging challenges for human society. It is commonly accepted that $CO_2$, as a greenhouse gas, is partly responsible for climate changes. It is thus important to reduce those $CO_2$ levels in every possible way. This can be achieved in different manners, for example by decreasing $CO_2$ emission by developing energy efficient processes with a reduced $CO_2$ emission or by capturing and storing the $CO_2$ that is still produced. A "greener" attitude will lower the ecological footprint help to decrease the $CO_2$ level.

The present PhD thesis focuses on one of those options, where $CO_2$ is separated and captured from gas mixtures produced by human activity. The capturing of $CO_2$ is established by means of the adsorption principle, where molecules are selectively trapped through their specific interaction with the surface atoms of a porous solid. The adsorbent materials studied in this work are part of the metal-organic framework (MOF) family. MOFs consist of metal ions or metal clusters, denoted as the nodes and organic compounds, denoted as the linkers. These metal clusters and organic linkers form 3 dimensional, crystalline networks with large surface areas wherein the $CO_2$ strongly adsorb.

A series of these MOFs with different features; framework flexibility, topology and functional groups are screened for their ability to adsorb $CO_2$ and $CH_4$. From these screening, one particular material, amino-MIL-53, a structure with amine groups anchored to its pore wall, was proven to be very selective in the separation of $CO_2$ from gas mixtures. This material was studied in closer detail. As a first study, pulse gas chromatographic analysis with different alkanes, branched and non-branched, alkenes and benzenes is performed. This gives a first impression of the nature of the adsorptive interactions in the material. Subsequently, the material is subjected to various techniques (breakthrough experiments, volumetric and gravimetric methods) to determine capacity and affinity for different gasses and the selective separation ability towards $CO_2$. Finally, the regenerability of the material is investigated as well as the performance in real adsorption cycles.