Thesis project: **Binders for sustainable concrete: modelling and predicting surface behavior**
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- Department: Process & Energy, 3mE
- Theme: Process Technology
- Is an external organization involved? TNO - Lab for Materials, Energy and Construction
- The thesis involves: Modeling (molecular dynamics)
- Prerequisite: programming skills (preferably Python),
  ideally also ME45211 Introduction to molecular simulation

In order for the building industry to become more sustainable, especially the cement production has to be reconsidered since it is responsible for more than 5% of the annual CO_2-emission worldwide. A promising way to reduce this footprint is by replacing traditional cement by alternative binders from secondary (aluminium-silica) materials such as fly ashes and blast furnace slag. However, these materials have as disadvantage that they do not spontaneously dissolve and harden when mixed with water like cement does. Instead, they have to be activated chemically. Although successful activators for the so-called geopolymer binders have been developed, these activators currently also have a high CO_2-footprint. In a drive to find a more sustainable activator, TNO has started a long-term investigation into the fundamental understanding of the dissolution and precipitation of Al-Si precursors such as fly ash and slag. Experimentally, we have some idea of which materials work well, but it is not fully understood why these materials work well. Molecular dynamics simulations are uniquely suitable to provide such microscopic insight to explain experimental observations and help to interpret measurements.

The goal of this project is to investigate the electric double layer around aluminium-silica materials such as slag and fly ashes with the ultimate purpose of developing sustainable building materials.