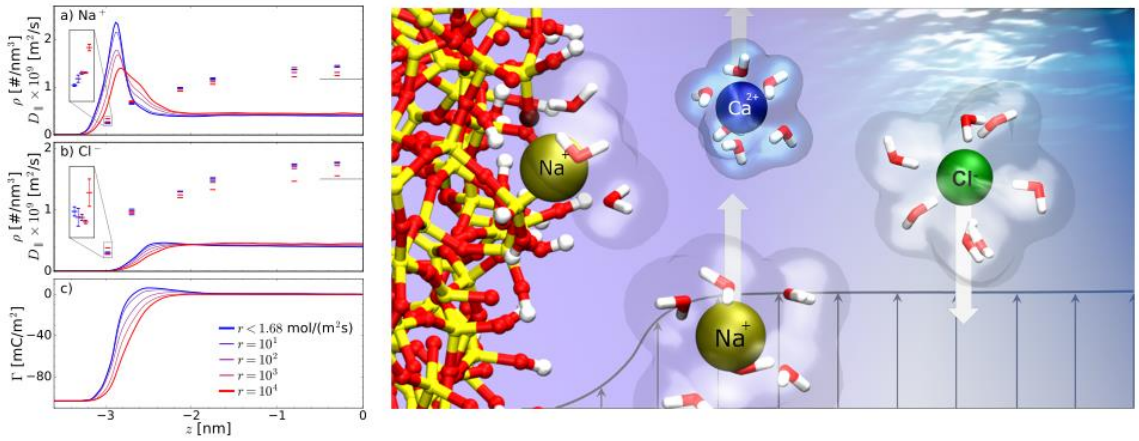
Thesis project: **Surface reaction kinetics affect adsorption and fluid flow**

Supervisor: dr. Remco Hartkamp (r.m.hartkamp@tudelft.nl)

- Department: Process & Energy, 3mE
- Theme: Process Technology (but also flow and energy)
- Is an external organization involved? No
- The thesis involves: Modeling (molecular dynamics)
- Prerequisite: programming skills (preferably Python),
  ideally also ME45211 Introduction to molecular simulation

Most solid materials will react when exposed to a watery solution, even if for no other reason than the acid-base reactions. Understanding this phenomenon is essential for biological systems, membranes, geology, sensors, and much more. While the solid reacts to the presence of the liquid, the opposite is also true, with the interfacial fluid properties being very sensitive to the details of the solid material, which is often considered as a homogenous flat surface in most experimental or modelling efforts.

In this project, you will use molecular dynamics simulation to explore how the much-overlooked surface reaction kinetics of a material has a far-reaching influence on the structure and transport of fluid along the surface. This project builds on the work of a previous master student, which has contributed to a recently published article [1]. A goal of the project is to improve upon the original method and measure how surface reaction rates affect the free energy that a nearby ion or molecule experiences.



References:

[1] M.F. Döpke, F. Westerbaan van der Meij, B. Coasne, and R. Hartkamp, 'Surface Protolysis and Its Kinetics Impact the Electrical Double Layer', Phys. Rev. Lett. **128**, 056001 (2022)