Thesis project: **Do micropores dominate electrode charging?**
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

Project description:

The use of porous electrodes is inextricably linked to a wide range of electrochemical processes for chemical conversion, energy application, or separation. Porous electrodes often consist of a combination of distinct micropores (< 2.5 nm) and macropores (> 50 nm). The micropores provide the material with a large specific surface area, whereas the macropores facilitate fast fluid transport to and from the micropores. Micropores have been reported to represent as much as 70% of the accessible surface area in activated carbon. This suggests that most ion adsorption occurs in these pores. However, the fluid transport in these pores do not simply adhere to traditional laws of fluid mechanics. In fact, the fluid properties are dominated by surface effects, which can lead to multiple orders of magnitude faster transport than predicted by conventional theoretical predictions. More so, the continuum assumption breaks down in pores below ~1 nm in diameter. Yet, current experimental and theoretical efforts related to porous electrodes are largely based on fitting global measurements in the context of continuum-based models. Such an approach does not respect the intricate multiscale physics that is responsible for the overall electrode performance. Consequently, predicting electrode performance or even tailoring of electrode materials is also currently difficult due to a lack of insight into the charging mechanics and ion transport within the electrode.

In this project, you will use constant surface potential molecular dynamics simulations of model micropores to investigate their charge dynamics with the aim to tailor the electrode properties and operating conditions for optimal performance.