

# Vacancy for 1 PhD student

## Solvent Design for CO<sub>2</sub> capture with molecular simulations

The Process and Energy (P&E) Department aspires to conduct world-class research and education focusing on process and energy technologies for sustainable development. The research is conducted from a deep understanding of the underlying physics and is oriented towards industrial applications and societal needs.

The work will be carried out in the Engineering Thermodynamics group of P&E. The project will be supervised by Dr.ir. Thijs J.H. Vlugt, in collaboration with the group of Prof. Joachim Gross in Stuttgart.

### Job Description

The project aims at the design of solvents for the capture of carbon dioxide, with a focus on low-pressure absorption/desorption processes. The solvents currently available for this purpose lead to a prohibitively high energy demand for cyclic processes. The objective of this work is to design solvents leading to energetically more favorable absorption and regeneration of the solvent.

We will use molecular simulations to study the reacting mixture (on a classical force field level), where finite concentrations are considered based on the quantum chemical calculations at infinite dilution. A correlation of the combined phase equilibrium and reaction equilibrium is subsequently done with state of the art equation of state models in order to allow for process optimization.

### Requirements

We seek candidates with an excellent MSc in the area of chemistry, physics, mathematics or computer science. Knowledge and experience in the fields of molecular simulation, numerical methods, or statistical mechanics would be advantageous but not necessary.

### Information and application

For more information about this position, please contact Dr.ir. Thijs J.H. Vlugt, [t.j.h.vlugt@tudelft.nl](mailto:t.j.h.vlugt@tudelft.nl)  
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