

# Vacancies for 3 PhD students and 1 postdoc

## Liquid Crystals as Absorption Liquids with a Solubility Switch

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 and Dr Th. de Loos, in collaboration with the group of Prof. Joachim Gross in Stuttgart. The project is financed by STW.

### Job Description

Liquid Crystals (LCs) are substances with a molecular ordering in between crystals and liquids. In a certain temperature range, the molecules show a crystal-like structure. Upon increasing temperature over a (sharp) phase transition temperature, however, this structure is broken and an (isotropic) liquid state is attained. This phase transition sharply changes the thermodynamic interaction with other components. The solubility of solutes, like carbon dioxide, in LCs changes step-wise over a very small temperature interval, much like a solubility-switch.

In this project, we will investigate this LC switch in detail. We are looking for 3 PhD students and 1 postdoc.

PhD1: This part of the project will focus on the experimental measurement of LCs+CO<sub>2</sub> phase equilibria. We aim at absorption processes of carbon dioxide in moderately dilute gas streams at elevated pressures (of up to 200 bar) and we are thus concerned with non-reacting or weakly reacting compounds. Our lab is equipped with phase equilibrium measurement facilities for any relevant pressure range (up to 4000 bar).

PhD2: This part of the project will focus on the development of a physically based equation of state, in order to describe the LCs+CO<sub>2</sub> phase equilibria. Ultimately, this equation of state will be used for optimal solvent design. This part of the project will be performed in close collaboration with Prof. Joachim Gross in Stuttgart.

PhD3: This part of the project will focus on classical molecular simulations to study phase equilibria of the LC+CO<sub>2</sub>. In particular, we will investigate in great detail why the solubility of CO<sub>2</sub> in nematic LC phases is so low. Simulations will also be used to understand the results of PhD1 and PhD2.

PD1: This part of the project will focus on the experimental synthesis of tailor-made LCs that will be used by PhD1.

## **Requirements**

We seek candidates with an excellent MSc in the area of chemistry or physics with some background in thermodynamics. For PhD2 and PhD3, knowledge and experience in the fields of molecular simulation, numerical methods, or statistical mechanics would be advantageous. For PD1, a strong background in organic synthesis will be required.

## **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) or Dr. Th. de Loos, [t.w.delooos@tudelft.nl](mailto:t.w.delooos@tudelft.nl).

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