SUPER – Stuttgart University Program for Experiencing Research
Project Information

Institute’s Information

Name of Institute: Institute of Thermodynamics and Thermal Process Engineering
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Duration of Project/Number of Students

June/July: x
June/July/August: x
Number of Students: 2

Name of Project: Application of classical density functional theory to interfacial phenomena

Beneficial Skills & Knowledge: Basic thermodynamics and applied mathematics, Programming experience (python or similar), linux basics

Description of Work

The objective of the project is the application and further development of a python program, in which classical density functional theory is implemented. Classical density functional theory is a powerful method used to describe inhomogeneous systems like phase boundaries. Combined with an equation of state like PC-SAFT, that is based on molecular properties, the concept can be used to predict interfacial properties for a wide range of substances.

The two applications we are interested in are adsorption processes and vapor-liquid interfaces. In adsorption processes, we want to calculate adsorption isotherms and investigate the influence of pore size. For fluid-liquid interfaces, we want to calculate surface tension of pure components as well as mixtures. In both cases the numerical results have to be validated by comparing them to experimental data.