Statistical mechanical modelling of the themophysical properties of complex fluids and materials

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A molecular description of matter is the key to understanding and predicting the properties of dense fluids and materials. The latest developments in statistical mechanical theories and computer simulation (Monte Carlo and molecular dynamics) are used in the Molecular Systems Engineering (MSE) group to provide a reliable predictive platform for complex fluids and ordered materials at the molecular level. The focus is on the phase equilibria of systems which are of industrial relevance, e. g., mixtures containing hydrogen fluoride (production of refrigerants), amines (processes for carbon capture), aqueous solutions of surfactants (enhanced oil recovery, structured phases), liquid crystals (optical devices), and active pharmaceutical ingredients (drug formulation and processing).