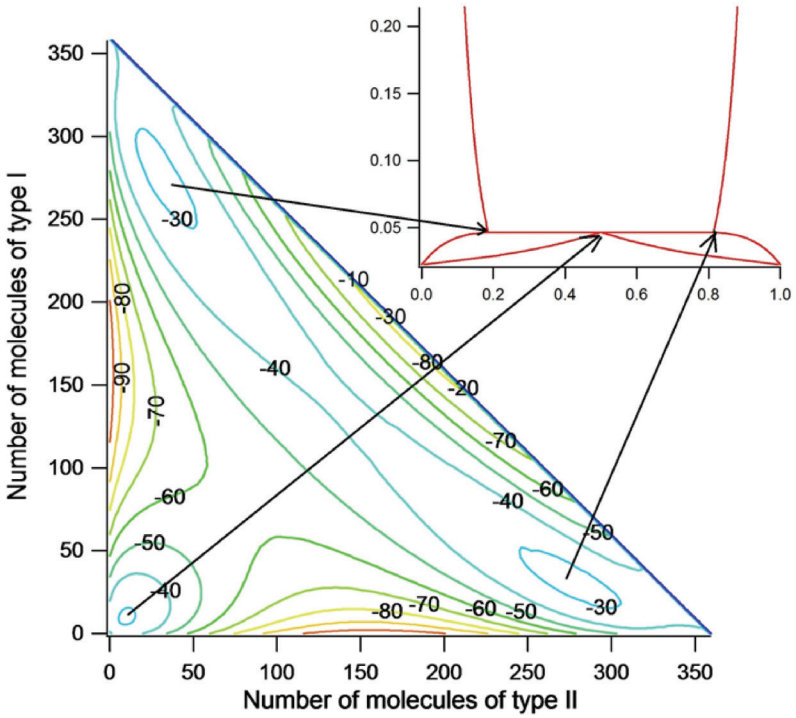
Molecular simulation study of phase equilibria of molecular fluids

In this work, we employ computationally efficient molecular simulation algorithms to study mixtures of molecular fluids. In literature, the traditionally employed simulation methods such as the Gibbs ensemble Monte Carlo technique require the knowledge of the phases in equilibrium a priori and computationally more expensive multi-box simulations.

Our present focus is on using alternate computationally efficient methods to determine the fluid phase equilibria of hydrocarbon mixtures. This data is necessary for the design and optimisation of process equipment, and is particularly useful in cases where limited experimental results are reported in literature. For example, many oxygen containing compounds (present in second generation biofuels) may decompose at elevated temperatures and hence, due to the challenges of performing experiments, molecular simulations are a cost effective alternate route to explore these systems.



Vapour-liquid-liquid equilibrium in a model binary mixture

Prof. Jhumpa Adhikari, Department of Chemical Engineering, adhikari@iitb.ac.in