







Mo 03.12.18 13:30 Uhr P 603

## Prof. Dr. Martin Oettel Universität Tübingen

## Phase transitions in lattice models with rodlike particles

We investigate phase transitions for hard rods with and without additional attractions on cubic lattices by simulation and theory. In 3D, grand canonical simulations show the occurrence of liquid-crystalline phases. The type of phases and the character of the transition are different compared to continuum models. Besides a standard nematic phase, a layered phase and a layered-nematic phase appear. For attracting rods, these transitions compete with the liquid-vapor transition and lead to (quasi-) tricritical points. Density functional theory for these lattice models can only reproduce some of the features seen by the simulations. We discuss the current strategy to obtain functionals and possible improvements.