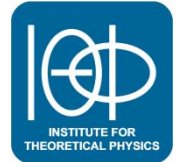




TECHNISCHE UNIVERSITÄT WIEN  
INSTITUT FÜR THEORETISCHE PHYSIK  
WIEDNER HAUPTSTRASSE 8-10, 1040 WIEN



## Invitation

Institute for Theoretical Physics – TU Wien

# Jürgen Horbach

Institut für Theoretische Physik II  
Heinrich-Heine Universität Düsseldorf, Germany

## From crystal nucleation to phase transitions in porous media: The role of interfacial free energies

### Abstract:

Material properties depend to a large extent on the interfaces that appear in their microstructure or that may form during solidification processes. Interfaces are also a central theme in the context of wetting phenomena at substrates and the phase behavior in porous media. Important quantities for the characterization of interfaces are interfacial free energies which are often hardly accessible from experiments. Here, I present novel methods to obtain interfacial free energies from particle-based computer simulations, using the analysis of capillary wave fluctuations, umbrella sampling and thermodynamic integration techniques. These methods are applied to a wide range of problems such as crystal nucleation in Nickel, various interfacial free energies between fluids/solids and substrates, and the phase behavior in porous media (colloid-polymer mixtures in confinement and the condensation of methane in metal-organic frameworks).

### Date:

Wednesday, **11.5.2016**, 13:00

### Venue:

Lecture hall – University Library  
TU Wien  
Resselgasse 4, 5th floor