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“Computing absolute free energies of disordered systems”

For most systems, free energies cannot be computed directly, as this task involves evaluation of an integral over phase space, which in general is not accessible. There is, however, a vast number of methods to compute free energy differences or derivatives. Hence, if a suitable reference system is known, one can access free energies of more complex systems via e.g. thermodynamic integration or similar procedures. For gases the ideal gas is a suitable reference, for crystals the harmonic crystal. For dense liquids, liquid crystals, membranes, solids with defect, etc, however, integration pathways would either involve first order phase transitions or they are long and hence prone to accumulation of error.

We present a computer simulation method, by which absolute free energies of dense, disordered systems can be computed.

We propose a scheme for the construction of reference systems, the free energy of which can be evaluated analytically, and which can be used to perform thermodynamic integration for e.g. membranes, liquid crystals or defects in solids.

Dienstag, 23. Februar 2010, 14.00 c.t.

Gebäude E2 6, Seminarraum E.04

Der Gast wird betreut von Ludger Santen (57411)

Alle Interessenten sind herzlich eingeladen.

Die Sprecher des Graduiertenkollegs
Manfred Lücke und Ludger Santen

**Strukturbildung und Transport
in komplexen Systemen**