

Physics seminar

Tuesday 10th may 2011 at 16h15
(coffee at 16h00)

Limpersberg
Room BS 1.04

Talk by Prof. Dr. Kurt Binder
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COMPUTER SIMULATIONS OF CRITICAL PHENOMENA AND PHASE BEHAVIOR OF FLUIDS

Computer simulation techniques such as Monte Carlo (MC) and Molecular Dynamics (MD) methods yield numerically exact information (apart from statistical errors) on model systems of classical statistical mechanics. However, a systematic limitation is the restriction to a finite (and often rather small) particle number N (or box linear dimension L , respectively). This limitation is particularly restrictive near critical points (due to the divergence of the correlation length of the order parameter) and for the study of phase equilibria possibly involving interfaces, droplets, etc.) Starting out with simple lattice gas (Ising) models, finite size scaling analyses have been developed to overcome this limitation. These techniques work for both simple Lennard-Jones fluids and their mixtures, including generalizations to approximate models for quadrupolar fluids such as carbon dioxide, benzene etc., and various mixtures, whose phase diagrams can be predicted. A combination of MC and MD allows the study of dynamic critical phenomena. Special techniques (Umbrella sampling plus thermodynamic integration) yield properties such as the surface free energies of droplets as function of droplet size. Thus, computer simulation has become a versatile and widely applicable tool for the study of fluids.

Next Physics Seminars

- **Tuesday, 24th May 2011:**
Belval, 16:15
Dr. German Olivares, UL
"Change detection analysis in geodesic time series"
- **Tuesday, 14th June 2011:**
Campus Limpertsberg, 16:15
Dominik Berg, UL
"The formation and characterization of kesterite thin film solar cells – challenges and solutions"
- **Tuesday, 28th June 2011:**
Belval, 16:15
Prof. Dr. M. Farle, U Duisburg-Essen
"Influence of nanoparticle shapes and morphologies on magnetic hardness"