On behalf of the

Science College CMS
Vienna Computational Materials Laboratory
and Center for Computational Materials Science

we cordially invite you to the following seminar

Mag. Georg Menzl

University of Vienna, Faculty of Physics, Computational Physics

Collective behaviour of single-file water chains in nanopore membranes

When a membrane of narrow carbon nanotubes is immersed in water, its pores are filled and the spatial confinement within the tubes leads to the formation of single-file water chains. These hydrogen bonded chains show ordering at room temperature such that the average dipole moment of the water molecules in the pores points along the tube axis. This order causes unique properties in comparison to bulk water, such as a large dielectric susceptibility and rapid proton transport along the water wires. We study membranes of parallel water wires by use of a dipole lattice model which allows the investigation of large systems and provides a physically transparent picture of the system. Our simulations show an order-disorder transition on square membranes and the critical temperatures for various pore lengths and pore spacings are obtained.

The influence of defects within the chains on system behavior is evaluated and we conclude that the chains, on average, are virtually defect-free for most lattices studied. We derive an analytic expression for corresponding states of a lattice of ordered chains which makes our simulation results applicable to a wide range of parameters. Analysis of the susceptibilities of square and triangular lattices shows the strong influence of inter-chain coupling on the dielectric response of the system thus providing a means of experimental verification via dielectric spectroscopy.

Date: Monday, Jan 24, 2011 16:00

Location: Seminar room 138C (TU Freihaus 9. Stock, gelb)
A-1040 Wien, Wiedner Hauptstaße 8-10