
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. Philipp Geiger

University of Vienna, Faculty of Physics, Computational Physics

Local Structure detection of polymorphic systems using neural networks

Distinguishing between different local structures is a complex computational problem of paramount importance for substances with rich phase diagrams. For instance, the study of crystallization of a supercooled liquid requires the detection of particles that are part of the growing crystal based only on local environment information.

Inspired by the use of feed forward neural networks to determine configurational energies, we use such networks in order to determine the structure around individual particles. Our novel method is simple, efficient and does not require the definition of a reference frame. This approach provides an order parameter for systems exhibiting complex crystal structures, such as high pressure ice phases, where conventional methods of classifying the system symmetry fail.

Date: Monday, Jan 24, 2011 16:00

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