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

## Dr. Eva González Noya

Instituto Química-Física Rocasolano, Madrid

# Phase behaviour of tetrahedral patchy particles

During the last few years the study of the phase behaviour of simple anisotropic models has attracted considerable attention. Much of this interest arose because several experimental groups have been able to produce anisotropic colloids and nanoparticles with much control over the anisotropy. These experiments open the possibility of building materials by self-assembly, i.e. by designing particles with specific shape and/or interactions that spontaneously assemble into a given target structure. In this respect, the study of the phase behaviour of simple anisotropic models will be very helpful to understand how the shape and interaction of the particles determines the formation of the desired structure.

One long time goal in this field is to produce particles with tetrahedral symmetry that assemble into a diamond crystal, which is motivated by its applications in photonics. As a first step to understand the factors that could lead to the appearance of low density solids and to study the mechanism for the nucleation we have studied the phase diagram of anisotropic particles with tetrahedral symmetry We will briefly discuss the available methods to calculate phase diagrams by computer simulations and present the results for the tetrahedral particles. Some preliminary studies about the kinetics of crystallization will also be discussed.

**Date:** Monday, March 14, 2011 16:00

**Location**: Josef-Stefan-Hörsaal,
Strudlhofgasse 4, 3rd floor, 1090 Wien