

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

Ms. Vera Batista

University of Cambridge, Department of Chemistry, Great Britain

Shape shifters: Crystallization and packing of deformable colloids

The interactions between colloidal particles can often be described by simple potentials, making many experimentally observed colloids amenable to investigation through analytic theory and computer simulation. In this talk I will address the effect of internal flexibility which is relevant to several types of colloids including globular proteins, micelles and emulsions. I will introduce and characterize a model for a generic class of colloidal particles that have a preferred shape but can undergo deformations while always maintaining hard-body interactions. The model consists of hard spheres that can continuously change shape at fixed volume into prolate or oblate ellipsoids of revolution, subject to an energetic penalty. The severity of this penalty is specified by a single parameter that determines the flexibility of the particles. The deformable hard spheres crystallize at higher packing fractions than rigid hard spheres, have a narrower solid–fluid coexistence region and can reach high densities by a second transition to an orientationally ordered crystal. I will also address the effect of flexibility on the packing properties of deformable ellipsoids of revolution.

Date: Monday, May 23, 2011 16:00
Location: Josef-Stefan-Hörsaal,
Strudlhofgasse 4, 3rd floor, 1090 Wien