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. Jonathan Yates

Department of Materials, University of Oxford, UK

First principles prediction of solid-state NMR parameters

Nuclear Magnetic Resonance can be a highly sensitive probe of atomic scale structure and dynamics in the solid-state. In recent years the planewave pseudopotential approach has been used to compute the key NMR parameters in diamagnetic solids (magnetic shielding, electric field gradients and indirect dipolar coupling).

I will outline the electronic origins of these NMR interactions. I will also try to convey the power (and limitations) of modern solid-state NMR, and the role calculations play in both the development and interpretation of novel NMR experiments. Applications will include nanomaterials and bio-inorganic compounds.

Date: Monday, March 21, 2011 16:00

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