# The 142<sup>nd</sup> iCeMS SEMINAR

#### Fri 04 October 2013 16:00-17:30

## Structural Transitions in Soft Porous Crystals Upon Fluid Adsorption: a Theoretical Approach

Lecturer:

### **Prof. Alain Fuchs**

Executive President Centre National de la Recherche Scientifique

#### Venue: 2nd Floor Seminar Room (#A207) iCeMS Main Building (#70), Kyoto University

Soft porous crystals are flexible metal-organic frameworks that respond to physical stimuli (temperature, pressure, and gas adsorption) by large changes in their structure and unit cell volume. I will describe a thermodynamic treatment, based on the so-called osmotic ensemble, of the interplay between guest adsorption and host deformation, where the bare host material can undergo elastic deformation, as well as structural transitions between metastable phases in the case of a multistable material. We show that in addition to structural transitions between metastable phases of bistable or multistable host frameworks, a new guest-stabilized host phase can be created when the size of the adsorbate is larger than the empty material's pore size. I will then confront the findings of our approach with experimental data for systems exhibiting phenomena such as gate opening and breathing.







