

Dear all,

**Nanoparticles by Design Unit (Sowwan Unit) would like to announce a seminar by Dr. Frank Abild-Pedersen, SUNCAT SLAC National Accelerator Laboratory.**

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**Date & Time: Thursday, October 2nd, 10:00-11:00**

**Venue: D014, Lab 1**  
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**Speaker: Dr. Frank Abild-Pedersen**

**SUNCAT SLAC National Accelerator Laboratory**

**Title: Concepts in Heterogeneous Catalysis -Application in the Syngas to Methanol Conversion**

**Abstract:** In the past decade the theoretical description of surface thermodynamics and kinetics has undergone a radical development. The important advances in density functional theory allows for a description of catalytic reactions at surfaces with the accuracy needed for computational results to compare directly with experiments. Computational methods such as DFT can be used to describe surface chemical reactions in detail and to understand variations in catalytic activity from one catalyst to another. In this presentation I will review the approach we have taken in recent years and how this approach applies towards the design of new catalysts. As a relevant example I will focus on the conversion of syngas to methanol, an important sub-reaction in the biomass to fuels process. I will also try to signify how such methods may be used in the future to engineer the electronic structure of the active surface by changing its composition and structure.

Host: Mukhles Sowwan, Nanoparticles by Design Unit

We look forward to seeing many of you.

Sincerely,

Yumi Takahashi

Nanoparticles by Design Unit (Sowwan Unit)