

Workshop on Neutron Methods for Probing the Science and Practice of Catalysis
Oak Ridge National Laboratory
September 16-17, 2010

ORNL is the World premier location for performing Neutron Science (<http://neutrons.ornl.gov/>) and has been involved in a number of events involving outreach to scientific communities. Examples include the Workshop on Imaging and Neutrons (2006) and the Dynamics of Soft Matter Workshop (2008). It is planned to hold a Workshop on *Neutron Methods for Probing the Science and Practice of Catalysis*. The goal of the workshops is to bring the heterogeneous catalysis and biocatalysis community together with experts in neutron science to discuss, explore and develop the possibilities for application of neutron methods to grand challenge problems in catalysis.

It is planned to hold 1 ½ day workshop that will begin with five sessions to explore the following subject areas

- Grand Challenges in Catalysis and related Neutron based methods
- Structural Characterization of catalysts under in situ conditions
- Probing dynamics of hydrogen on catalysts and in molecules by incoherent scattering
- Dynamics of molecules and catalysts by coherent inelastic neutron scattering
- Biocatalysis
- Modeling in neutron experiments

It is planned to have two speakers in each session who will first outline and describe a selection of challenging problems in catalysis in each of the subject areas and second describe how existing or planned neutron techniques and instruments might be used to address these problems. In each session the talks will be followed by an extensive discussion and Q&A session. On the second day, there will be breakout sessions aimed to allow all participants an opportunity to describe their own research aspirations and to discuss with other participants how they might apply neutron methods to achieve their own goals. The discussion of the proceedings of the meeting will be captured in a Workshop report and it is intended that the speaker's presentations will be summarized in a journal publication. By the end of the Workshop the participants should have the vision and knowledge to prepare their own beamline proposal for performing experiments at the High Flux Isotope Reactor (HFIR) or the Spallation Neutron Source (SNS). Proof of principle catalysis experiments using neutrons will be identified that would be awarded beamtime in summer-fall 2010. Plans will be initiated for a related session at future American Chemical Society annual meeting.

The Workshop will be held at the Central Laboratory Office (CLO) building at the ORNL SNS during User week (Sep 13-17), a joint event hosted by the SNS and ORNL's Center for Nanophase Material Sciences (CNMS). The confluence of these events will provide a unique opportunity for participants to first visit and learn about these two interconnected User Centers and attend tutorial workshops on neutron instrumentation and measurement, immediately prior to the Workshop, held on Sep 16 and 17.

The Workshop is sponsored by the ORNL Neutron Sciences and Physical Sciences Directorates, the Joint Institute for Neutron Sciences, the Oak Ridge Associated Universities,

the FIRST Energy Frontier Research Center, and by DOE-BES-Chemical Sciences. It is scientifically associated with ORNL's Center for Nanophase Materials Sciences.

The Scientific Organizing Committee includes
Steve Overbury, ORNL, chair
Takeshi Egami, University of Tennessee and ORNL
Dean Myles, ORNL
Vivianne Schwartz, ORNL
Peter Cummings, ORNL
Phil Britt, ORNL
Leighton Coates, ORNL
Ken Herwig, ORNL
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