

**Neutrons for Catalysis: A Workshop on Neutron Scattering Techniques for Studies in Catalysis**  
 Oak Ridge National Laboratory, Spallation Neutron Source, Building 8600  
 September 16-17, 2010, Iran Thomas Auditorium, Room A-103

<b>Thursday, September 16, 2010</b>	
7:15 am	Shuttle bus leaves Comfort Inn hotel
7:30	Registration; Breakfast available (Atrium)
8:00	<b>Introduction and Program Overview</b> <ul style="list-style-type: none"> <li>• Michelle Buchanan, Oak Ridge National Laboratory</li> <li>• Pappannan Thiagarajan, US DOE</li> </ul>
8:10	<b>Meeting Grand Challenges in Catalysis through Neutron Scattering Techniques</b> Moderators: Phil Britt, Ken Herwig <i>Each presentation will be 30 minutes with 10 minutes Q&amp;A</i> <ul style="list-style-type: none"> <li>• Bruce Gates, University California at Davis, “Grand challenges in catalysis research: understanding catalysis at the atomic scale as a basis for design of catalytic structures”</li> <li>• Juergen Eckert, University of California, Santa Barbara, “Neutrons as microscopic probes in heterogeneous catalysis”</li> </ul>
9:30	Break (Atrium)
9:45	<b>Probing Dynamics of Molecules in Catalysts Systems by Inelastic Neutron Scattering</b> Moderators: Steve Overbury, David Wesolowski <i>Each presentation will be 30 minutes with 5 minutes Q&amp;A.</i> <ul style="list-style-type: none"> <li>• Peter Stair, Northwestern University, “Some Thoughts About Surface Hydroxyl Groups and Catalysis”</li> <li>• Peter Albers. AQura, “Applications of Neutron Scattering and Chemical Industry Characterizations of Technical Catalysis from Operating Large Scale Plants, Hydrogen Species on Fuel Cell Catalysis”</li> <li>• Eugene Mamontov, Oak Ridge National Laboratory, “What can we learn about the mobility of species in catalytic systems using quasielastic neutron scattering?”</li> </ul> Discussion follows (40 minutes)
12:10 pm	Lunch and open discussion (Atrium)
1:00	<b>Structural Characterization of Catalysts and Catalytic Materials</b> Moderators: Viviane Schwartz, Takeshi Egami <i>Each presentation will be 30 minutes with 5 minutes Q&amp;A</i> <ul style="list-style-type: none"> <li>• J. van Bokhoven, ETH Zurich, “Shining light on catalysts”</li> <li>• Thomas Proffen, Los Alamos National Laboratory, “Advanced Characterization of Materials using Total Scattering”</li> </ul> Discussion follows (40 minutes)
2:50	Break (Atrium) and Group Photo
3:00	<b>Probing Biocatalysis by Neutron Scattering Methods</b> Moderator: Dean Myles. <i>Each presentation will be 30 minutes with 5 minutes Q&amp;A</i> <ul style="list-style-type: none"> <li>• Robert Blankenship, Washington University of St. Louis, “Neutron Scattering Studies of Photosynthetic Energy Transduction Complexes”</li> <li>• Paul Langan, Los Alamos National Laboratory. “Neutrons for biocatalysis”</li> </ul> Discussion follows (30 minutes)
4:40	<b>Break-out Session I – Attacking Grand Challenge problems with neutron experiments</b> <ul style="list-style-type: none"> <li>• Structure (SNS Iran Thomas Auditorium): Breakout facilitator: Mike Simonson, Breakout spokesman: Henry Lamb, Scribes: Viviane Schwartz, Ashfia Huq</li> <li>• Dynamics (SNS Room C-152); Breakout facilitator: Phil Britt, Breakout spokesman: Rob Rioux, Scribes: Michelle Kidder</li> <li>• Biocatalysis (SNS Room C-464): Breakout facilitator: Dean Myles, Breakout spokesman: Andreas Bommarius, Scribes: Leighton Coates</li> </ul>
6:30	<b>Reception, Dinner, and Tour of SNS (Atrium)</b>
8:30	<b>Buses depart SNS for hotel (SNS flagpole)</b>

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**Iran Thomas Auditorium (Room A-103), Spallation Neutron Source, Building 8600**  
**Oak Ridge National Laboratory**  
**Friday, September 17, 2010**

7:15 am	Buses depart hotel
7:30	Breakfast available (Atrium)
8:00	<p><b>Results of Break-out Session I</b></p> <ul style="list-style-type: none"> <li>• Dynamics (Robert Rioux, Pennsylvania State University) (10 minutes)</li> <li>• Structure (Henry Lamb, North Carolina State University) (10 minutes)</li> <li>• Biocatalysis (Andreas Bommarius, Georgia Institute of Technology) (10 minutes)</li> </ul> <p><i>Clarification and Q&amp;A (10 minutes)</i></p>
8:40	<p><b>Modeling of Catalysts, Catalysis and Neutron Experiments; A crosscutting activity</b></p> <p>Moderators: Peter Cummings, Bobby Sumpter. <i>Each presentation will be 30 minutes with 5 minutes Q&amp;A</i></p> <ul style="list-style-type: none"> <li>• David Sholl, Georgia Institute of Technology, “Combining theory and neutron scattering to understand molecular diffusion in porous solids”.</li> <li>• A.J. Ramirez-Cuesta, ISIS Facility, STFC, Rutherford Appleton Laboratory, “The Power of Inelastic Neutron Scattering: Vibrational Spectroscopy of hydrogen - applications to catalysis”</li> </ul> <p><i>Discussion follows 20 minutes</i></p>
10:10	<p><b>Discussion of proposal preparation</b></p> <p>Dean Myles</p>
10:20	<p><b>Break-out Session II – P-o-p experiments, proposal preparation, crosscutting activities</b></p> <ul style="list-style-type: none"> <li>• Structure (<i>SNS Iran Thomas Auditorium</i>): Breakout facilitator: Mike Simonson, Breakout spokesman: Henry Lamb, Scribes: Viviane Schwartz</li> <li>• Dynamics (<i>SNS Room C-156</i>): Breakout facilitator: Phil Britt, Breakout spokesman: Rob Rioux, Scribes: Michelle Kidder</li> <li>• Biocatalysis (<i>SNS Room C-152</i>): Breakout facilitator: Dean Myles, Breakout spokesman: Andreas Bommarius, Scribes: Leighton Coates</li> </ul>
12:00 pm	<b>Lunch, Closing Remarks and Wrap-up</b> (SNS Iran Thomas Auditorium)
1:00	<p><b>CNMS Discovery Seminar</b> (SNS Iran Thomas Auditorium)</p> <p>Simon Bare, UOP, LLC, “Development and Applications of an Program for in situ XAFS Studies for Catalyst Characterization at UOP”</p>
2:00	<p><b>Discussion of Workshop published output</b> (SNS Room C-156)</p> <p>Speakers, spokesmen, facilitators (invitation only)</p>
2:10-5:00	<p><b>Preparation of Workshop Summary Report</b> (SNS Room C-156)</p> <p>Session facilitators, spokesmen, scribes, others (invitation only)</p>