

## The Theory and Practice of Catalysis

**Organizers:** Horia Metiu and Fabio Ribeiro

**July 6 – 10, 2015**

**TSRC Host:** Mark Kozak 970-708-4426, mark@telluridescience.org

**Location:** Telluride Elementary School, 447 West Columbia Avenue, Telluride

### Monday July 6

8:30 am	Breakfast at TSRC meeting site	
9:00 am	Horia Metiu and Fabio Ribeiro, welcome and announcements	
<i>morning session chair: Jeffrey T. Miller</i>		
9:15 am	Hajo Freund	Models for heterogeneous catalysts: Complex materials at the atomic level
10:15	break	
10:45 am	Carl Mesters	C1 chemistry & catalysis for the energy supply
11:45 am	discussion, then lunch on your own	
<i>afternoon session chair: Hans Niemantsverdriet</i>		
1:30 pm	Robert Schlögl	Structure function relation in selective oxidation catalysis
2:30 pm	Israel Wachs	The dynamics of surface metal oxide catalysts under reaction conditions
3:30 pm	break	
3:45 pm	William Schneider	Operando DFT computations applied to NO <sub>x</sub> catalysis
4:45 pm	discussion, then adjourn	

### Tuesday July 7

8:30 am	Breakfast at TSRC meeting site	
<i>morning session chair: William Schneider</i>		
9:00 am	Hans Niemantsverdriet	Fischer-Tropsch synthesis in gas and coal to liquids technology: How surface science and model catalysts can help
10:00 am	break	
10:30 am	Jeffrey T. Miller	In situ synchrotron characterization of alloy NPs for alkane dehydrogenation
11:30 am	discussion, then lunch on your own	
<i>afternoon session chair: Carl Mesters</i>		
1:30 pm	Robert Rioux	Bulk intermetallics: A platform for selective hydrogenation and the development of multinuclear single-site catalysts
2:30 pm	Bruce Gates	Molecular metal catalysts with crystalline zeolite and MOF supports as ligands
3:30 pm	break	
3:45 pm	Dario Stacchiola	Tuning the properties of copper-based catalysts based on In-situ studies of model systems

4:45 pm	discussion, then adjourn
6:00 pm	Town Talk, Conference Center in Mountain Village

### Wednesday July 8

8:30 am	Breakfast at TSRC meeting site	
<i>morning session chair: Dario Stacchiola</i>		
9:00 am	Horia Metiu	Alkane catalysis by modified oxides
10:00 am	break	
10:30 am	Michael Bowker	Practical and model catalysts for methanol selective oxidation
11:30 am	Eric W. McFarland	Oxyhalogenation: Light alkane conversion without carbon dioxide
12:30 pm	lunch on your own followed by traditional joint hike	
6:00 pm	Picnic, Telluride Elementary School, 447 West Columbia Avenue	

### Thursday July 9

8:30 am	Breakfast at TSRC meeting site	
<i>morning session chair: Bruce Gates</i>		
9:00 am	Jeroen van Bokhoven	Dynamical structure of catalysts
10:00 am	break	
10:30 am	Aditya Bhan	Be practical: Mechanistic studies of industrially relevant catalytic systems
11:30 am	discussion, then lunch on your own	
<i>afternoon session chair: Michael Bowker</i>		
2:00 pm	Peter Stair	Single-site catalysis in oxidation and C-H activation
3:00 pm	break	
3:30 pm	Alexander Katz	New organic-inorganic interfaces for enhancing catalysis on solid surfaces
4:30 pm	discussion, then adjourn	

### Friday July 10

8:30 am	Breakfast at TSRC meeting site	
<i>morning session chair: Aditya Bhan</i>		
9:00 am	Johannes Lercher	TBA
10:00 am	break	
10:30 am	Fabio Ribeiro	Exploring the catalytic landscape of Cu/SSZ-13 using NO oxidation and standard selective reduction of NO with NH <sub>3</sub>
11:30 am	wrap-up discussion	
noon	adjourn	