## 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		
morning session chair: Jeffrey T. Miller			
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		
afternoon session chair: Hans Niemantsverdriet			
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**

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8:30 am	Breakfast at TSRC meeting site		
morning session chair: William Schneider			
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		
afternoon session chair: Carl Mesters			
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		
0.00 pm			

### Wednesday July 8

8:30 am	Breakfast at TSRC meeting site			
morning session chair: Dario Stacchiola				
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			
morning session chair: Bruce Gates				
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			
afternoon session chair: Michael Bowker				
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	
morning session chair: Aditya Bhan		
9:00 am	Oliver Gutierrez	Elementary steps during hydrogenation, hydrotreating and
		nucleophilic substitution on sulfide-based catalysts
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 $NH_3$
11:30 am	wrap-up discussion	
noon	adjourn	