

***Tentative schedule for the TSRC Workshop  
Metal-organic Frameworks: Experiments and Simulations***

**Organizers:** Shengqian Ma, Omar Farha, Brian Space, Francesco Paesani

**TSRC Hosts:** Mark Kozak (970-708-4426) and Kristen Redd (970-708-0827)

**Meeting Location:** Telluride Elementary School, 477 West Columbia Telluride CO 81435

**Dates:** June 14- 18, 2015

**All breakfasts are at the Telluride Elementary School and are provided, for participants only, by TSRC**

**All invited talks are 45 minutes long including discussions and questions**

**Sunday, June 14**

- 8:30 am - 9:00 am: Breakfast at TSRC
- 9:00 am - 11:00 am: Badge Pick-Up
- 6:30pm: Dinner together

**Monday, June 15**

- 8:30 am - 9:00 am: Breakfast at TSRC
- 9:00 am - 9:15 am: Welcome by organizers & TSRC
  - 9:15 am - 10:00 am: Omar Farha  
*Catalytic Metal-Organic Framework*
  - 10:00 am - 10:45 am: David Sholl  
*Computationally screening MOF for real applications: how close are we to the dream?*
- 10:45 am - 11:00 am: Coffee Break
  - 11:00 am - 11:45 am: David Harris  
*Isolation and study of reactive heme species in metal organic frameworks*
  - 11:45 am - 12:30 am: Jian Zhang

*Indium Porphyrin Frameworks: An Efficient Photocatalytic Platform for Organic Synthesis*

- 12:30 pm - 2:00 pm: Lunch in Town
  - 2:00 pm - 2:45 pm: Myoung Soo Lah  
*Hollow metal-organic frameworks: a metal-organic polyhedron single crystal as a sacrificial template*
  - 2:45 pm - 3:15 pm: Jeremy Klosterman  
*Exploiting MOFs for Functional Chromophore Assemblies*
- 3:15 pm - 3:30 pm: Coffee Break
  - 3:30 pm - 4:15 pm: Ognjen Miljanic  
*MOFs without metals*
  - 4:15 pm - 5:00 pm: Shengqian Ma  
*Task-Specific Functionalization of Porous Organic Polymers*

**Tuesday, June 16**

- 8:30 am - 9:00 am: Breakfast at TSRC
  - 9:00 am - 9:45 am: Hong-Cai Zhou  
*Preparation of Robust Metal-Organic Frameworks for Practical Applications*
  - 9:45 am - 10:30 am: Francesco Paesani  
*New computational tools for modeling metal-organic frameworks*
- 10:30 am - 10:45 am: Coffee Break
  - 10:45 am - 11:30 am: Vitalie Stavila  
*MOF-Based Catalysts for Selective Hydrogenolysis of Carbon-Oxygen Bonds in Aromatic Ethers*
  - 11:35 am - 12:15 pm: Stephen FitzGerald  
*Infrared Spectroscopy of H<sub>2</sub> in MOFs*
- 12:15 pm - 1:45 pm: Lunch in town
  - 1:45 pm - 2:30 pm: Mircea Dinca  
*Redox reactivity and catalysis enabled by cation exchange at MOF SBUs*
  - 2:30 pm - 3:15 pm: Wonyoung Choe  
*Expandable Metal-Organic Frameworks with Rotary Hinges*

- 3:15 pm - 3:30 pm: Coffee Break
  - 3:30 pm - 4:15 pm: Brian Space  
*MOM MODELING -- TODAY AND TOMORROW*
  - 4:15 pm - 5:00 pm: Craig Brown  
*Structural studies of small molecules in MOFs*
  
- 6:00 pm – 7:15 pm: ***TSRC Town Talk at the Conference Center in Mountain Village***

### **Wednesday, June 17**

- **Free Day**
- **Group Hike (TBA)**
- **6:00 pm – 9:00 pm:** TSRC Picnic under the tent at the Elementary School  
(Family and guests welcome free of charge)

### **Thursday, June 18**

- 8:30 am - 9:00 am: Breakfast at TSRC
  - 9:00 am - 9:45 am: Krista Walton  
*Post-synthetic metal insertion in metal-organic frameworks for enhanced ammonia adsorption from air*

**Meeting Adjourns by Noon**