

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

Organizers: Seth Cohen, Shengqian Ma, Francesco Paesani, Brian Space

TSRC Hosts: Nana Naisbitt (970-708-0004) and Rory Sullivan (970-708-4542)

Meeting Location: Telluride Intermediate School, 725 W. Colorado

Dates: July 7- 11, 2014

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

All invited talks are 45 minutes long including discussions and questions

Monday, July 7

- 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 Materials
 - 10:00 am - 10:45 am: Tom Woo
The MOF Mating Game, Machine Learning and Other Computational High Throughput Screening Tools
- 10:45 am - 11:00 am: Coffee Break
 - 11:00 am - 11:45 am: Shengqian Ma
Tailoring Metal-Organic Frameworks as Nanoreactors
 - 11:45 am - 12:30 pm: Karl Johnson
Carbon Dioxide Capture and Conversion in Metal Organic-Frameworks
- 12:30 pm - 2:00 pm: Lunch in Town
 - 2:00 pm - 2:45 pm: Mark Allendorf
Emergent Properties Using the Guest@MOF Concept
 - 2:45 pm - 3:30 pm: Rochus Schmid
MOF-FF - A First Principles Parametrized Force Field for Structure and Dynamics of Flexible MOFs

- 3:30 pm - 3:50 pm: Coffee Break
 - 3:50 pm - 4:35 pm: Myoung Soo Lah
Postsynthetic Modifications of Metal–Organic Frameworks: Framework Ligand Exchanges, Insertions and Deletions
 - 4:35 pm - 5:20 pm: Hani El-Kaderi
Gas Separation by Nitrogen-Rich Porous Organic Polymers

Tuesday, July 8

- 8:30 am - 9:00 am: Breakfast at TSRC
 - 9:00 am - 9:45 am: Mircea Dinca
Intrinsic Charge Transport in MOFs
 - 9:45 am - 10:30 am: Padmini Ramaswamy
Proton Conductivity in MOFs: Challenges and Opportunities
- 10:30 am - 10:50 am: Coffee Break
 - 10:50 am - 11:35 am: Guillaume Maurin
Adsorption & Diffusion in Hybrid Porous Materials: Molecular Simulations in Synergic Combination with Experiments
 - 11:35 am - 12:20 pm: Francesco Paesani
Water Dynamics and Proton Transport in MOFs
- 12:20 pm - 2:00 pm: Lunch in town

- **6:00 pm – 7:15 pm: TSRC Town Talk at the Conference Center in Mountain Village**

Wednesday, July 9

- 4:00 pm - 4:45 pm: Nathaniel Rosi
Core-SHell MOFs
- 4:45 pm - 5:30 pm: Maciej Haranczyk
Exploring Frontiers of the Material Space of Metal-Organic Frameworks
- 5:30 pm - 6:15 pm: J.R. Schmidt
Ab Initio Physically-Motivated Force Fields for MOFs
- **6:00 pm – 9:00 pm:** TSRC Picnic @ Ah Haa School for the Arts, 300 S. Townsend
(Family and guests welcome free of charge)

Thursday, July 10

- 8:30 am - 9:00 am: Breakfast at TSRC
 - 9:00 am - 9:45 am: Jeffrey Long
Gas Separations in Metal-Organic Frameworks
 - 9:45 am - 10:30 am: Michael Zaworotko
Hybrid Organic-Inorganic Materials for Carbon Capture
- 10:30 am - 10:50 am: Coffee Break
 - 10:50 am - 11:35 am: Brian Space
Potentials that Work for MOF Simulations: Past, Present & Future
 - 11:35 am - 12:20 pm: Kostantinos Vogiatzis
Ab Initio Modeling of Gas Adsorption and Catalysis in MOFs
- 12:20 pm - 2:00 pm: Lunch in town
 - 2:00 pm - 2:45 am: Brian Smith
Covalent Organic Frameworks from Homogenous Conditions: Systematic Manipulation and Mechanistic Insights
 - 2:45 pm - 3:30 pm: Jeffrey Greathouse
Comparing MOF Properties Between Simulation and Experiment
- 3:30 pm - 3:50 pm: Coffee Break
 - 3:50 pm - 4:35 pm: Nour Nijem
Spectroscopic Methods to Probe Guest Interactions in MOFs

Friday, July 11

- 8:30 am - 9:00 am: Breakfast at TSRC
 - 9:00 am - 9:45 am: Adam Matzger
Porosity: Too Much, Too Little, and Just Right
 - 9:45 am - 10:30 am: Seth Cohen
MOFs as Support Matrices for Biomimetic Catalysts

Meeting Adjourns by Noon