TSRC Workshop: Advanced Methods for De Novo Prediction of Chemical Reaction Networks
Organizers: Bill Green (MIT) and Jim Pfaendtner (University of Washington)

List of participants/institutions and workshop venue available here:
https://www.telluridescience.org/meetings/workshop-details?wid=619

Schedule:

	Monday July 25 (mostly PES-based methods)
8:00 - 9:00	Breakfast (Telluride Elementary School
9:00 - 9:15	Bill+Jim: Meeting over/welcome
9:15 - 10:00	Bill: “Predicting Complex Reaction Networks: Why and How”
10:00 - 10:45	Carlo: "A Systematic Approach To Investigate Potential Energy Surfaces of Reacting Systems"
10:45 - 11:15	Break
11:15 - 12:00	Karl: "Searching Potential-Energy Surfaces of Molecules"
12:00 - 1:15	Lunch + group hikes (there will be a few options plans to return to rooms by 4:00)
1:15 - 2:00	
2:00 - 3:30	
3:30 - 4:15	
4:15 - 5:00	
5:00 - 5:45	Paul: "Searching for Reaction Networks using Strings and Graphs"
5:45 - 6:30	Yury: "Automated Discovery of Elementary Chemical Reaction Steps by Combining Freezing String and Berny Optimization Methods with the Bond Electron Matrix Representation"

Note: the afternoon break is to encourage small group discussions and informal interactions. We will propose a few options for lunch as well as a few different options for potential hikes. Any needed information / advance planning will be shared at least the week before the workshop.

	Tuesday July 26 (mostly graph theory based methods)
8:00 - 9:15	Breakfast
9:15 - 10:00	Richard: TBD
10:00 - 10:45	Franklin: "Automatic Mechanism Generation In Heterogeneous Catalysis"
10:45 - 11:15	Break
11:15 - 12:00	Judit: "KinBot, an autonomous reaction path explorer for elementary reactions"
12:00 - 1:15	Lunch
1:15 - 2:00	Dimitrij: "Predicting Feasible Organic Reaction Pathways Using Heuristically-Aided Quantum Chemistry"
2:00 - 3:30	Break
3:30 - 4:15	Linda: "Unraveling Complex Catalytic Chemistries through Reaction Pathway Analysis"
4:15 - 5:00	Group / panel discussion on standards for validating methods
5:00 - 5:45	***Telluride town talk***
5:45 - 6:30	

	Wednesday July 27 (mostly MD-based methods)
8:00 - 9:00	Breakfast
9:15 - 10:00	Jim: "Molecular Dynamics Based Approaches for Enumerating Reaction Topology and Kinetics "
10:00 - 10:45	David: "Accelerated molecular configuration space searching using the boxed molecular dynamics method "
10:45 - 11:15	Break
11:15 - 12:00	Group discussion (topic TBD) // afternoon lunch and/or group hike
12:00 - 1:15	
1:15 - 2:00	
2:00 - 3:30	
3:30 - 4:15	Birgit: "Transition networks for understanding protein self-assembly"
4:15 - 5:00	Graeme: "Computational methods for simulating long time scales and for catalyst design"
5:00 - 5:45	***TSRC Wed evening picnic / dinner (included with registration)***
5:45 - 6:30	