## The Theory and Practice of Catalysis

Organizers: Horia Metiu, Eric McFarland

July 25 – 28, 2022

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

Location: Telluride Intermediate School, 725 West Columbia Avenue, Telluride

### **Monday July 25**

| 8:30 am                                  | Breakfast at TSRC meeting location |  |  |  |
|--|------------------------------------|--|--|--|
| 9:00 am                                  | welcome and announcements          |  |  |  |
| morning session chair: Eric W. McFarland |                                    |  |  |  |
| 9:15 am                                  | Aditya Bhan                        | Kinetics with site ensembles, branched networks, and         |  |  |
|  |                                    | multiple kinetically relevant steps                          |  |  |
| 10:15 am                                 | break                              |  |  |  |
| 10:30 am                                 | Charles T. Campbell                | Particle size and support effects on the energetics of metal |  |  |
|  |                                    | nanoparticles, and correlations between these energetics     |  |  |
|  |                                    | and catalyst performance                                     |  |  |
| 11:30 am                                 | discussion, then lunch on your own |  |  |  |
| afternoon session chair: Aditya Bhan     |                                    |  |  |  |
| 1:30 pm                                  | Vanda Glezakou                     | Global optimizers, large scale simulations and enhanced      |  |  |
|  |                                    | sampling for catalysis problems                              |  |  |
| 2:30 pm                                  | break                              |  |  |  |
| 2:45 pm                                  | Yong Wang                          | Earth abundant Fe-based catalysts for hydrodeoxygenation     |  |  |
| 3:45 pm                                  | discussion, then adjourn           |  |  |  |

### **Tuesday July 26**

| 8:30 am                                    | Breakfast at TSRC meeting location   |  |  |  |
|--|--|--|--|--|
| morning session chair: Charles T. Campbell |  |  |  |  |
| 9:00 am                                    | Horia Metiu  | Hydrogen production without CO <sub>2</sub>        |  |  |
| 10:00 am                                   | break  |  |  |  |
| 10:15 am                                   | Rajamani Gounder   | Altering Zeolite Properties to Influence Rates and |  |  |
|  |  | Selectivities of Alkene and Aromatics Reactions    |  |  |
| 11:15 am                                   | discussion, then adjourn   |  |  |  |
| 6:30 pm                                    | Town Talk, The Telluride Depot, 300 S Townsend Street                        |  |  |  |
|  | Viewpoints Matter: How diverse perspectives bring about scientific progress  |  |  |  |
|  | Korana Burke, University of California Davis; Peter Salamon, San Diego State |  |  |  |
|  | University; Dontarie Stallings, University of California San Diego           |  |  |  |

# Wednesday July 27

| 8:30 am                                    | Breakfast at TSRC meeting location                                   |  |  |  |
|--|--|--|--|--|
| morning session chair: Phillip Christopher |  |  |  |  |
| 9:00 am                                    | Eric W. McFarland  | Affordable Green"ish" Production of Hydrogen From            |  |  |
|  |  | Fossil Resources   |  |  |
| 10:00 am                                   | break  |  |  |  |
| 10:15 am                                   | Simon Bare   | Identifying The Active Site in Catalysis: What is the future |  |  |
|  |  | for synchrotron methods?                                     |  |  |
| 11:15 am                                   | discussion, followed by lunch on your own and traditional joint hike |  |  |  |
| 5:30pm                                     | Picnic at The Depot, 300 S. Townsend St.                             |  |  |  |

# **Thursday July 28**

| 8:30 am                                | Breakfast at TSRC meeting location |   |  |  |
|--|------------------------------------|---|--|--|
| morning session chair: Rajmani Gounder |                                    |   |  |  |
| 9:00 am                                | Phillip Christopher                | Tuning the reactivity of atomically dispersed metal     |  |  |
|  |                                    | catalysts: Bifunctional pair sites and UV photolysis    |  |  |
| 10:00 am                               | break                              |   |  |  |
| 10:15 am                               | Matteo Cargnello                   | Understanding and Engineering Catalytic Materials Using |  |  |
|  |                                    | Nanocrystal Precursors                                  |  |  |
| 11:15 am                               | discussion, then adjourn           |   |  |  |