



UNIVERSITY OF CALIFORNIA, MERCED

ccCAT Retreat January 17, 2020

Primary Location: GRAN 120

- 9:00 am Welcome
ACS Chemistry Colloquy Space
Light breakfast fare will be provided.
- 9:40 am Introduction and Retreat Overview
- 9:50 am Lightning Talks (Yue Yu, Vince Aguirre, Shao-Yu Lu, Md. Mehdi Masud, Remi Leano)
- 10:20 am Lightning Talks (Rijan Karkee, Karnamohit Ranka, Hanbo Hong, Christian Sarabia, Bradford Barker)
- 10:50 am Break
- 11:00 am Workshop: Compiling software on MERCED: a case study with Octopus. (David Strubbe)
Preparation: be sure to have MERCED account
- 12:00 pm Lunch
ACS Chemistry Colloquy Space
Lunch will be provided.
- 1:30 pm Lightning Talks (Ali Abou Taka, Ajay Khanna)
- 1:45 pm Workshop: Using the Atomic Energy Network (aenet) package for machine-learning molecular properties (Tim Zuehlsdorff)
- 2:30 pm Break
- 2:40 pm JCTC Planning (Hrant Hratchian)
- 3:20 pm Break
- 3:30 pm Workshop: Introduction to concepts from physics education research (Bradford Barker)
- 4:20 pm Closing Reception
ACS Chemistry Colloquy Space