Workshop Schedule

Sunday, June 9
3:00 - 5:00 – Check-In, Photo/Badge
5:30 - 6:30 – Dinner
6:30 - 7:00 – Welcome & Staff Introductions & Rules
7:00 - 7:30 – Ice-Breakers
7:30 - 9:30 – Scavenger Hunt

Monday, June 10
7:30 – Breakfast
8:30 – Announcements, Check-In, Photo/Badge
9:00 – 9:15 – Welcome and Introduction to MolSSI
9:15 - 10:15 – Introduction to Electronic Structure Theory
10:15 - 10:30 – Break
10:30 - 11:30 – Application and Opportunities in Electronic Structure Research
11:30 - 12:30 – Lunch
12:30 - 1:30 – Python Session 1: Using Jupyter, Introduction, file parsing
1:30 - 4:00 – Python Session 2: Working with multiple files, tabular data
4:00 - 5:00 – Group Session
5:00 - 5:30 – Roses and Thorns
5:30 - 7:00 – Dinner
7:00 - 9:00 – Open

Tuesday, June 11
7:30 – Breakfast
8:00 – Announcements
9:00 - 10:15 – Python Session 3: Data visualization and graphics
10:15 - 10:30 – Break
10:30 - 11:30 – Introduction to Molecular Dynamics
11:30 - 12:30 – Lunch
12:30 - 1:30 – Applications and Opportunities in Molecular Dynamics Research
1:30 - 4:00 – Python Session 4: Writing functions, running code from the command line
4:00 - 5:00 – Group Session

5:00 - 5:30 – Roses and Thorns
5:30 - 7:00 – Dinner
7:00 - 9:00 – Open

Wednesday, June 12
7:30 – Breakfast
8:00 – Announcements
8:30 - 9:00 – Group Photo
9:00 - 10:30 – Python Session 5: Sharing code on Github, building a python module with CC
10:30 - 10:45 – Break
10:45 - 12:00 – CMS Session 1: Modeling vibrational motion using ab initio methods
12:00 – 1:00 – Lunch
1:00 - 2:00 – Enhancement Speaker: Richard Tapia, Rice University Professor
2:00 - 4:00 – CMS session 2: calculation of potential energy surface using psi4; spline fitting to the PES
4:00 - 5:00 – Group Session
5:00 - 5:30 – Roses and Thorns
5:30 - 7:00 – Dinner
7:00 - 9:00 – Open/Movie

Thursday, June 13
7:30 – Breakfast
8:00 – Announcements
9:00 - 10:30 – CMS session 3: Differentiation of the spline to get gradients and forces; discussion of the importance of these quantities to Newton's laws of motion

10:30 - 10:45 – Break
10:45 - 12:00 – CMS session 4: Using the Velocity Verlet method to solve Newton's equations of motion on the computer
12:00 – 1:00 – Lunch
1:00 - 2:00 – Enhancement Speaker: Angel Marti, Rice University Professor

2:00 - 4:00 – CMS session 5: Application of the velocity-verlet method to PES, analyzing and animating vibrational trajectories

4:00 - 5:00 – Group Presentation Prep
5:00 - 5:30 – Roses and Thorns
5:30 - 6:30 – Dinner
6:30 - 7:00 – Physical Activity
7:00 - 8:30 – Group Presentation Prep
8:30 - 9:30 – Talent show

Friday
7:30 – Breakfast
8:00 - 9:00 – Check out
9:00 - 10:00 – Practice/Finalize slides for student presentation
10:00 - 12:00 – Student Presentation
12:00 - 1:00 – Lunch/Talk by Dr. Tapia
1:00 - 3:30 – Industry Enhancement Speakers
3:30 - 4:00 – Group Photo and Goodbyes
4:30 – Depart