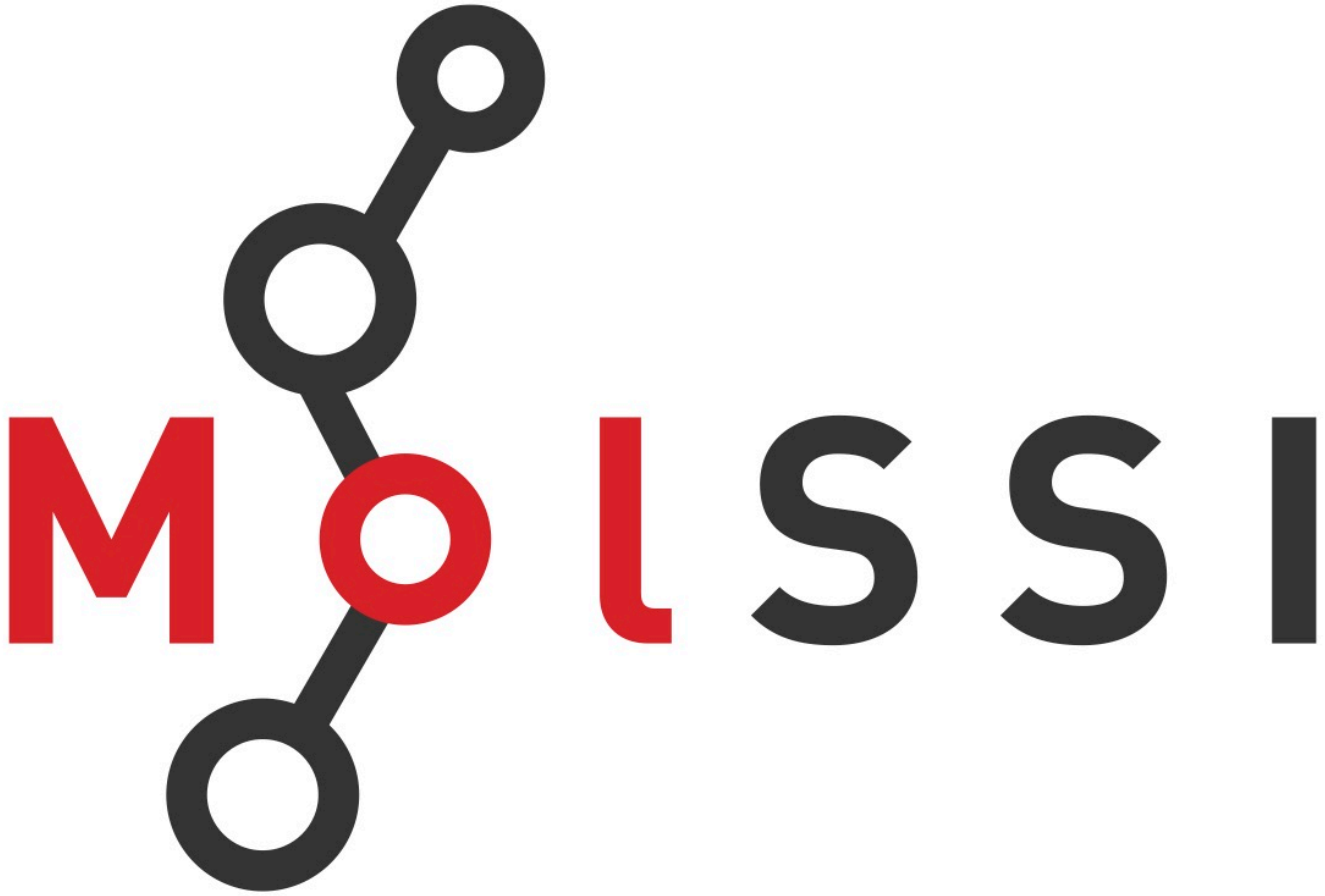



# Berkeley MSSE Bootcamp

Information Session

June 25, 2020

# The Molecular Sciences Software Institute

The Molecular Sciences Software Institute serves as a nexus for science, education, and cooperation serving the worldwide community of computational molecular scientists, a broad field including of biomolecular simulation, quantum chemistry, and materials science.

- Funded by the National Science Foundation starting in 2016.
- Collaborative effort between 8 PIs. Currently 8 faculty members on Board of Directors and 10 full time Software Scientists.

3 Broad Goals:

1. To provide community education and leadership
2. To provide software infrastructure.
3. To provide education and training.

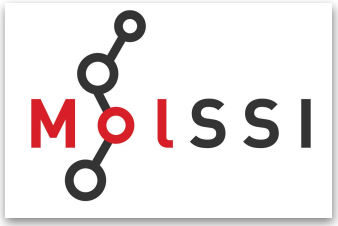
MolSSI

# Who is MolSSI

MolSSI

# MolSSI Software Projects

- COVID-19 Hub - community-driven data repository and curation service for molecular structures, models, therapeutics, and simulations
- QCArchive - Compute, store, and analyze large amounts of quantum chemistry data
- QCSchema - Common input and output format for quantum chemistry
- MM Interoperable Components - A pipeline agnostic API for MM and MD methods to encapsulate the human expertise into swappable parts
- Basis Set Exchange - Website and Python library for obtaining and manipulating basis sets
- MolSSI Driver Interface (MDI) - standardized API for fast, on-the-fly communication between computational chemistry codes
- SEAMM - Simulation Environment for Atomistic and Molecular Modeling. User-friendly environment for CMS, providing building, simulation, and analysis tools.
- Quantum Chemistry Machine Learning Datasets - Commonly-used datasets freely-available for download in multiple formats

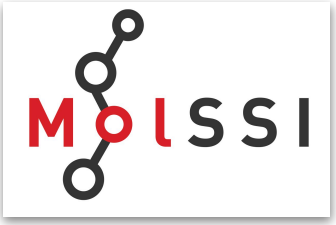



# MolSSI Education

Broad Goal: Provide training on coding and software development to undergraduate students, graduate students, post docs, and faculty in the molecular sciences.

Approach: Hands on workshops and projects. Guided instruction modeled after Software Carpentry.

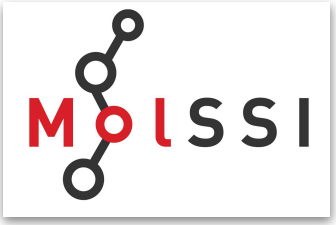
MolSSI Education holds multiple training programs, workshops and bootcamps around the US (and sometimes internationally) each year.




# MSSE Bootcamp Goals

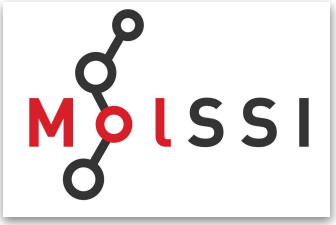
Our goal in the bootcamp is to...

- establish good software development practices - version control, code collaboration, unit testing, clean coding style.
- develop coding skills - development environments, understand python and C++ code, differences between languages.
- apply knowledge to computational chemistry - create a simple monte carlo and/or molecular dynamics code.




# MSSE Bootcamp Project

- Collaborate in your team to create a simple Monte Carlo and/or Molecular Dynamics code.
  - In Python
  - In C++
- Apply software development principles.




# MSSE Bootcamp Structure

The bootcamp will consist of two parts, guided instruction and a group project.

- Guided instruction: There will be 2-3 hours of live, guided, instruction each day on the selected topic.
- Group project: You will be expected to work with your group each day to apply concepts from the guided instruction to your project.