**Introduction to Molecular Simulations in Python**

**Instructor: Meghana Munipalle**

**Registration link: NA**

**Approximate duration: 4 hours**

**Prerequisites:**

* Basic Python knowledge: syntax, file I/O
* Access to Google Colab

**Summary:**

This workshop will introduce molecular simulation, a powerful type of modeling with applications in many fields, including chemistry, biology, physics, medicine, and more. The theory behind two common forms of molecular modeling, molecular dynamics (MD) and Monte Carlo (MC), will be reviewed, and we will use Python to set up, run, and analyze these two types of simulations.

**Contents:**

1. **Introduction to Molecular Simulation (30 min)**
   1. The Ergodic Theorem
   2. Statistical Mechanics- Averaging
2. **Monte Carlo (MC) Simulations (1.5 hr)**
   1. Basics of MC (45 min)
      1. The Boltzmann distribution
      2. The MC Algorithm
      3. What does a MC simulation tell us?
   2. Hands-on: Performing an MC simulation in Python (45 min)
3. **Molecular Dynamics (MD) Simulation (1.5 hr)**
   1. Basics of MD (45 min)
      1. Force Fields
      2. The MD Algorithm
      3. What does a MD simulation tell us?
   2. Hands-on: Performing an MD simulation in Python (45 min)
4. **Analyzing Molecular Simulations in Python (30 min)**
   1. Hands-on: Using ML to analyze MD trajectories