2/11/2020 Week 5 Module 1
Molecular Mechanics and Molecular Dynamics

- This module will consist of a
  - mini-lecture on molecular mechanics and molecular dynamics
  - walk-through of a python script to run molecular dynamics with OpenMM
- At the end of this module, you should be able to address these questions:
  - What is molecular mechanics and why do people use it instead of quantum mechanics?
  - Generally speaking, how does a molecular dynamics simulation work?
- You should also be able to run a molecular dynamics simulation of a simple system using OpenMM

What is Molecular Mechanics?

- Quantum mechanics
  - given the coordinates of atomic nuclei, provides the best description of a system's energy
  - computationally expensive and currently infeasible for biomolecules
- Molecular mechanics
  - treats atoms as hard spheres
  - empirical potential energy
- QM/MM
  - treats part of a system with QM and most with MM
  - in many applications, may balance accuracy and computational speed

- See 1st 45 seconds of "An Introduction to Molecular Dynamics" (https://www.youtube.com/watch?v=lLFEqKl3sm4)