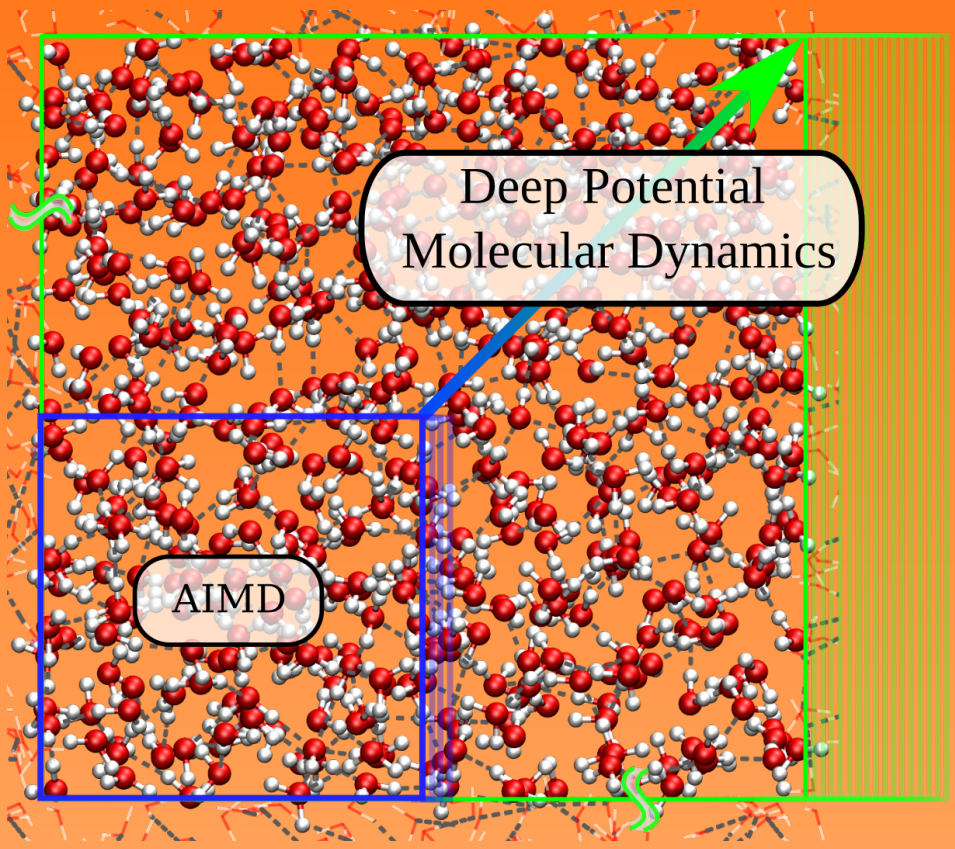
Molecular Simulation with Machine Learning

July 13-14, 2020, Princeton University, Princeton, NJ USA



Speakers:

S. Baroni (SiSSA)
M. Ceriotti (EPFL)
R. DiStasio (Cornell)
M. Fernandez-Serra (SUNY)
G. Grest (Sandia)
G. Kresse (U. Vienna)
T. Kuhne (U. Paderborn)
P. Piaggi (Princeton)
W. E (Princeton)

Schedule:

Date: July 13-14, 2020
Location: Lewis Library, Room 120

A two-day workshop covering theory and hands-on tutorials on the software package for molecular simulation with machine learning (ML) tools developed at the Computational Chemical Science Center "**Chemistry in Solution and at Interfaces**" (chemlabs.princeton.edu/ccsc/). The package includes codes to construct and use deep neural network models of the potential energy surface and electronic properties of multi-atomic systems that reproduce the results of electronic density functional theory.

ML codes need interfacing with community codes for electronic structure and ab-initio simulation, classical molecular dynamics, path-integral molecular dynamics, and enhanced sampling of rare events. The workshop will pro-mote discussions on how to better achieve code integration within the molecular simulation community across disciplines ranging from physical chemistry to condensed matter physics and materials science. The workshop will include general presentations, panel discussions, and tutorial sessions.

Application forms are available on the workshop website: http://chemlabs.princeton.edu/ccsc/upcoming-events/. The number of participants is limited. The deadline for application is May 15, 2020. Accepted participants should pay a registration fee of 100 USD, which includes the meals. Partial financial support for students and post-docs may be available.

Contact information:

Clarice Gethers-Mubarak (cgethers@princeton.edu)

U.S. DEPARTMENT OF ENERGY
Chemistry in Solution and at Interfaces
Computational Chemical Science Center
CENTER FOR STATISTICS AND MACHINE LEARNING
PRINCETON UNIVERSITY