LAMMPS (Large-Scale Atomic/Molecular Massively Parallel Simulator)

This page provides links to various nanoHUB resources related to LAMMPS (Large-Scale Atomic/Molecular Massively Parallel Simulator).

The [Polymer Modeler tool], powered by LAAMPS, builds thermoplastic polymer chains and run LAMMPS to relax the chains and study mechanical properties.

The [Atomic Stick-Slip tool], powered by LAMMPS, enables users to easily perform non-equilibrium molecular dynamics simulations of the atomic stick-slip that occurs between an atomic force microscope tip and substrate, and then analyze their simulation results quantitatively.

The [Nano Heatflow tool], powered by LAMMPS, studies the transfer of energy between the vibrational modes of a carbon nanotube.