

**Assignment #1**  
Due 10/14/15

Please prepare the assignment in the form of a technical report describing the calculations made (including any relevant equations), followed by the results. For the first assignment, you should be able to make extensive use of the examples provided from the LAMMPS website as templates for your calculations. Post questions on GoPost when practical.

1. Calculate the bulk and Young's modulus of Stillinger-Weber silicon. Calculate the Young's modulus of a thin Si nanobeam and compare to the Young's modulus of bulk SW silicon. Comment on the implications for NEMS. Generate a model for the behavior of nanobeams as function of cross-sectional dimensions. Analyze how the yield stress of a nanobeam depends on the strain rate.
2. Calculate the energy versus radius of Au nanoparticles using EAM potential. Compare to continuum theory based on a fixed surface energy.
3. Using EAM potential, put a single Cu adatom on an fcc Cu 111 surface. Run MD to calculate surface diffusivity as function of temperature (use temperature range accessible with moderate run-times, e.g., near melting point).
4. Use MD to calculate something of interest to you.