Hands-On-Session –II on Monday 23/01/12 Time 2-4pm

Complete the assignments of Lab Session-I.

Make a new copy of your Pot. Energy Program & Name it "loginid_2a.c" (retain your older version!!)

- 1. Read the fcc (4x4x4) positions (x, y, z already generated)
- 2. Read in a cut_off distance from I/P
- 3. Impose PBC & Minimum Image Convention
- 4. Calculate Pot. Energy U for different cutoff distances (Rc); (Find U for Rc=4.0 to 10 Å in steps of 0.5 Å)

Bring Your Notebooks/C/Fortran-books;

Do not use internet!