The Chinese University of Hong Kong

PHYS4061 Computational Physics, 1st semester, 2019-2020

Project A Part IV

Write a subroutine of Steepest Decent and Conjugate Gradient method for minimization of total energy. Test these methods by randomly displacing atoms (very small displacements) in LJ (50%) based crystal and the crystal structure of your choice in part 4, and then relaxing the atoms to their equilibrium positions.

(Hint: try 2 atoms scenario to test the minimization before try it on lattice)

Plot the starting and the ending positions of your crystal structures using VMD. You may get 10% bonus if you implement CG in SW/Tersoff or EAM potentials, but your total score is capped at 100%

Due date: 10th Dec,2019

Score will be deducted if the submission is late.

Please submit this lab to Prof. Zhu email jyzhu@phy.cuhk.edu.hk