The Chinese University of Hong Kong

PHYS4061 Computational Physics, 1st semester, 2019-2020

Project A Part III

1. (30%) Write a subroutine for total energy calculation implementing the Lennard-Jones potential.
2. (70%) Write a subroutine for total energy calculation implementing one of the following potentials at your preference:
    a. EAM potential for metals,
    b. SW or Tersoff potential for Si, or
    c. Coulomb potential for ionic solids with Buckingham potential.

    You need to apply PBC to all the vector and distance calculations. If you choose a or b, you'll get 10% bonus, however the total score is capped at 100%. Attention, the optimization of a or b can be considerably difficult. If you find that you can't finish lab 4 on a or b, you can also try c in lab 4, which is relatively simpler. Your bonus won't be deducted in this part.

    You can check your result by: 1. Converging average energy per atom when increasing periodicity. 2. Same energy contribution among all atoms. 3. Lowest energy lattice constant match with literatures. (See detail in the updated powerpoint)

You need to check literatures for all the related parameters. Also make sure to include your references in your report. Submit to ylfchong@phy.cuhk.edu.hk , use this as title of email :"Lab3 submission (Full name) (SID)". Please put your work inside a compressed folder named like this:" lab3_(fullname)_(SID).zip/rar".

Due date: 22 Oct 2019

Score will be deducted if the submission is late.