MDI 505 Homework 3

Spring 2019

Due February 26, 2019 by 3:30p

Modify the code we developed in the notes for calculating the energy versus spacing curve for an fcc solid to model a bcc structure. Compare energetics for both fcc and bcc at the equilibrium as a function of the cutoff distance. While the code in class was in MatLab, you should convert the code and submit in .ipynb format.

Note: as you increase the cutoff, you must increase the number of cells in the sum.