First Principle 2017-Fall Homework 3 Solution

Kai-Hsin Wu (吳愷訢)*
Department of Physics and Center of Theoretical Sciences, National Taiwan University, Taipei 10607, Taiwan

1. The following shows the result of Al and Na:

- Al

(1) a_0 using volume optimization:

$$a_0 = 4.05000$$

(2) Variation with different a_0:

a_0	E
3.90	-14.541085
3.95	-14.665726
4.00	-14.735369
4.05	-14.757538
4.10	-14.738699
4.15	-14.684395
4.20	-14.599834

(3) the following figure shows the energy (E) v.s. V :

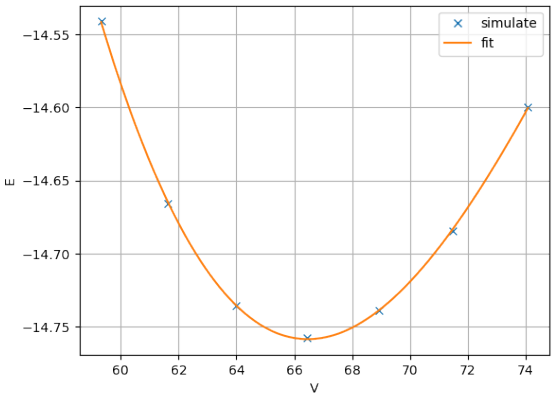

FIG. 1. Al-fcc E-V

* r05222003@ntu.edu.tw

By using third order polyfit, and with the following formula, we can get the bulk-modulus B and the minimum a_0:

$$B = V\frac{\partial^2}{\partial V^2}E$$
$$V = a_0^3$$

$$a_0 = 4.050723 \ \ \mathring{A}$$
$$B = 74.608739 \ \ GPar$$

(4) We start with HF energy density and seek for the minimum of r_s :

$$e^{HF} = \frac{2.21}{r_s^2} - \frac{0.916}{r_s}$$

Where the unit of energy is Ry and r_s is in unit of bohr radius. The minimum is at :

$$r_s = 2.553467 \ \ \mathring{A}$$

using following relation by which we consider 1-free electron per unit-cell, we can estimate the lattice constant a_0 :

$$\frac{4\pi}{3}r_s^3 = n^{-1}$$
$$\frac{N_{free}}{a_0^3} = n$$

$$a_0 = \left(\frac{4\pi}{3}\right)^{1/3} r_s$$
$$\approx 4.11616 \ \ \mathring{A}$$

- Si
