

First Principle 2017-Fall Homework 3 Solution

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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 :

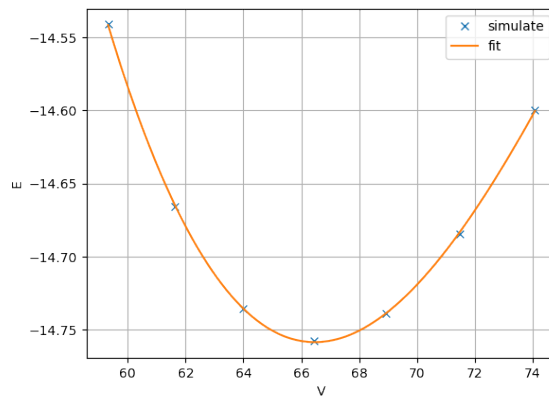


FIG. 1. Al-fcc E-V

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

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

$$V = a_0^3$$

$$a_0 = 4.050723 \text{ \AA}$$

$$B = 74.608739 \text{ GPar}$$

(4) Consider the free electron HF energy density and seek for the minimum of r_s :

$$e^{HF} = \frac{A}{r_s^2} - \frac{\beta}{r_s}$$

$$A = 2.21$$

$$B = 0.916$$

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

$$r_s^* = \frac{2A}{\beta}(\text{bohr}) = 2.553467 \text{ \AA}$$

using following relation by which we consider 4 free electrons per unit-cell, we can estimate the lattice constant a_0 :

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

$$\frac{N_{free}}{a_0^3} = n$$

$$a_0 = \left(\frac{16\pi}{3} \right)^{1/3} r_s$$

$$\approx 6.1737 \text{ \AA}$$

For Bulk modulus, we have following relation. by which we express Ω in terms of r_s :

$$\frac{N}{\Omega} = n = \frac{3}{4\pi r_s^3}$$

$$B = \Omega \frac{\partial^2 E}{\partial \Omega^2}$$

$$= \frac{1}{12\pi r_s} \left[\frac{-2}{r_s} e^{HF'} + e^{HF''} \right]$$

$$= \frac{1}{6\pi r_s^4} \left[\frac{5A}{r_s} - 2\beta \right]$$

we have the bulk modulus at r_s^*

$$B = \frac{\beta^4}{6\pi(2A)^4} \frac{\beta}{2} (Ry/bohr^3)$$

$$\approx 18.468 GPa$$

- Na

