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:

$a_0(\AA)$	$E(eV)$
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 :

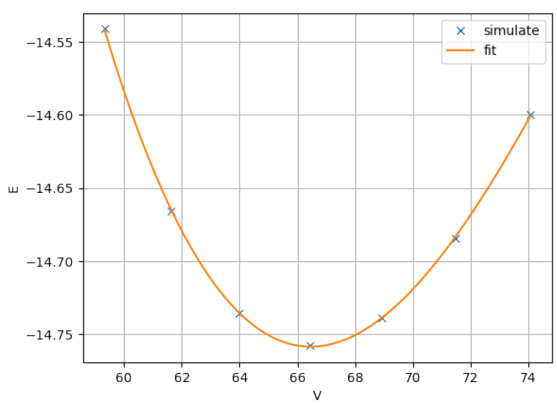

FIG. 1. Al-fcc E-V

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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:

$$
\begin{aligned}
B &= V\frac{\partial^2}{\partial V^2}E \\
V &= a_0^3
\end{aligned}
$$

$$
\begin{aligned}
a_0 &= 4.050723 \ \ \mathring{A} \\
B &= 74.608739 \ \ GPa
\end{aligned}
$$

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

$$
\begin{aligned}
e^{HF} &= \frac{A}{r_s^2} - \frac{\beta}{r_s} \\
A &= 2.21 \\
B &= 0.916
\end{aligned}
$$

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

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

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

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

$$
\begin{aligned}
a_0 &= \left(\frac{16\pi}{3}\right)^{1/3} r_s \\
&\approx 6.1737 \ \ \mathring{A}
\end{aligned}
$$

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

$$
\begin{aligned}
\frac{N}{\Omega} &= n = \frac{3}{4\pi r_s^3} \\
B &= \Omega\frac{\partial^2 E}{\partial \Omega^2} \\
&= \frac{1}{12\pi r_s}\left[\frac{-2}{r_s}e^{HF'} + e^{HF''}\right] \\
&= \frac{1}{6\pi r_s^4}\left[\frac{5A}{r_s} - 2\beta\right]
\end{aligned}
$$

we have the bulk modulus at r_s^*

$$
\begin{aligned}
B &= \frac{\beta^4}{6\pi(2A)^4}\frac{\beta}{2}(Ry/bohr^3) \\
&\approx 18.468 GPa
\end{aligned}
$$

- Na

(1) a_0 using volume optimization:

$$a_0 = 4.05000$$

(2) Variation with different a_0:

$a_0(\mathring{A})$	$E(eV)$
3.9241059	-1.437731
3.9645606	-1.443730
4.0050153	-1.447706
4.0454700	-1.449866
4.0859247	-1.449972
4.1263794	-1.448133
4.1668341	-1.445039
4.2072888	-1.440498

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

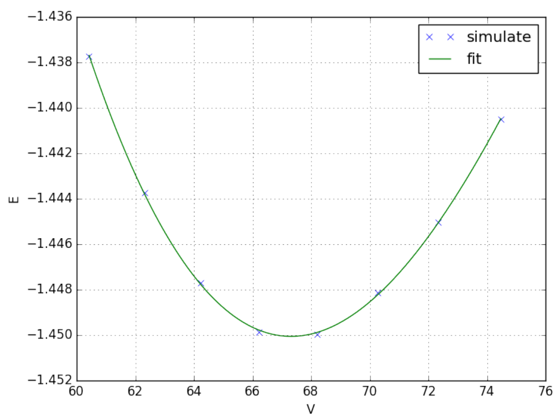

FIG. 2. Na-fcc E-V

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

$$
\begin{aligned}
B &= V\frac{\partial^2}{\partial V^2}E \\
V &= a_0^3
\end{aligned}
$$

$$a_0 = 4.06802437 \;\; \mathring{A}$$
$$B = 4.83347453 \;\; GPa$$

(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 :

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

using following relation by which we consider 2 free electrons per unit-cell, we can estimate the lattice constant a_0 :

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

$$a_0 = \left(\frac{8\pi}{3}\right)^{1/3} r_s$$
$$\approx 5.186047 \;\; \mathring{A}$$

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^*

$$B = \frac{\beta^4}{6\pi (2A)^4} \frac{\beta}{2} (Ry/bohr^3)$$
$$\approx 18.468 GPa$$