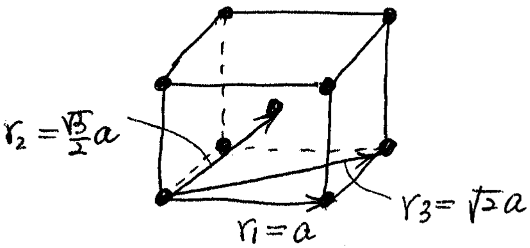
1 $\psi(r) = V_0 \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right]$, $V_0 = 0.09$ eV/atom, $\sigma = 3.9$ Å



6 nearest neighbor of $r_1 = a$

8 " " $r_2 = \frac{\sqrt{3}}{2}a$

12 " " $r_3 = \sqrt{2}a$

$$\mathcal{E} = \frac{1}{2}\sum \psi(r) = \frac{V_0}{2}\left[6\left\{\left(\frac{\sigma}{a}\right)^{12} - \left(\frac{\sigma}{a}\right)^{6}\right\} + 8\left\{\left(\frac{\sigma}{a}\right)^{12}\left(\frac{2}{\sqrt{3}}\right)^{12} - \left(\frac{\sigma}{a}\right)^{6}\left(\frac{2}{\sqrt{3}}\right)^{6}\right\} + 12\left\{\left(\frac{\sigma}{a}\right)^{12}\left(\frac{1}{\sqrt{2}}\right)^{12} - \left(\frac{\sigma}{a}\right)^{6}\left(\frac{1}{\sqrt{2}}\right)^{6}\right\}\right]$$

$$= V_0 \left\{ 25.5684 \left(\sigma/a\right)^{12} - 13.2315 \left(\sigma/a\right)^6 \right\}$$

$\partial\mathcal{E}/\partial a = 0$; $25.5684\,\sigma^{12} \times (-12)\,a^{-13} - 13.2315\,\sigma^6 \times (-6)\,a^{-7} = 0$.

$$\rightarrow \boxed{a = 1.25270\,\sigma = 4.8856 \text{ Å}}$$

$$\mathcal{E}^\circ = \frac{V_0}{2}\left[6\left\{1.25217^{-12} - 1.25217^{-6}\right\} + 8\left\{1.25217^{-12}\left(\frac{2}{\sqrt{3}}\right)^{12} - 1.25217^{-6}\left(\frac{2}{\sqrt{3}}\right)^{6}\right\} + 12\left\{1.25217^{-12}\left(\frac{1}{\sqrt{2}}\right)^{12} - 1.25217^{-6}\left(\frac{1}{\sqrt{2}}\right)^{6}\right\}\right]$$ with $V_0 = 0.09$

$$\therefore \boxed{\mathcal{E}^\circ = -0.154 \text{ eV/atom}}.$$

2 $\psi(r) = V_0 \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right]$

(a) 2 first nearest neigbors of $r_1 = a$

2 second " " $r_2 = 2a$

$$\rightarrow \boxed{\begin{aligned}\mathcal{E} &= \frac{1}{2}\sum \psi(r) = \frac{V_0}{2}\left\{2\times\left[\left(\frac{\sigma}{a}\right)^{12} - \left(\frac{\sigma}{a}\right)^{6}\right] + 2\times\left[\left(\frac{\sigma}{2a}\right)^{12} - \left(\frac{\sigma}{2a}\right)^{6}\right]\right\} \\ &= V_0\,\frac{\sigma^6\left(4097\sigma^6 - 4160a^6\right)}{4096\,a^{12}} = V_0\left[1.000\times\left(\frac{\sigma}{a}\right)^{12} - 1.016\left(\frac{\sigma}{a}\right)^{6}\right].\end{aligned}}$$

(b). $\partial\mathcal{E}/\partial a = 0$;

$$\frac{\partial\mathcal{E}}{\partial a} = V_0\left\{\sigma^{12}(1+2^{-12})(-12)a^{-13} - \sigma^6(1+2^{-6})(-6)a^{-7}\right\} = 0$$

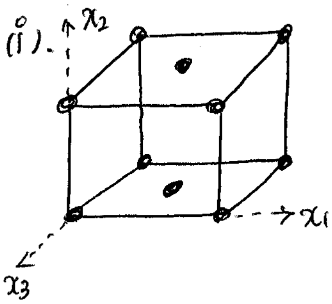
$$\therefore \boxed{a_0 = \left(\sqrt[6]{\frac{(1+2^{-12})}{(1+2^{-6})}\cdot 2}\right)\cdot\sigma \approx 1.1196\,\sigma.}$$

3

For solving the problem;

The Bravais lattice, or space lattice, is an infinite array of points, determined by the lattice vectors $\mathbf{R}$, where $\mathbf{R} = n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2 + n_3 \mathbf{a}_3$ such that every n_i is an integer. The $\mathbf{a}$'s are the three primitive vectors of the Bravais lattice: in three dimensions, they must have a non-zero $\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)$ product. There are infinite number of different choices for the primitive vectors of a given lattice.

(i).

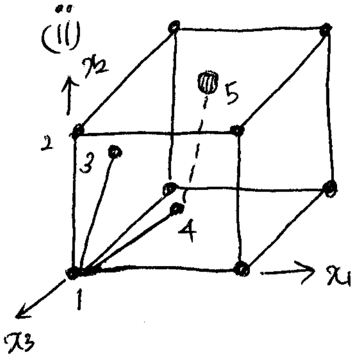


$\boxed{\text{It is a Bravais Lattice}}$.

Because, lattice vectors can be expressed as:

$$\boxed{\begin{aligned} \mathbf{a}_1 &= \frac{a}{2}(\mathbf{e}_1 + \mathbf{e}_3) \\ \mathbf{a}_2 &= \frac{a}{2}(\mathbf{e}_1 - \mathbf{e}_3) \\ \mathbf{a}_3 &= a\mathbf{e}_2 \end{aligned}}$$

(ii)



$\boxed{\text{It's not a Bravais Lattice}}$.

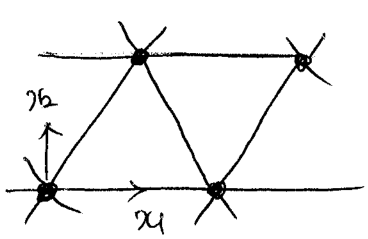
Let's assume that we found lattice vector to reach to all atoms:

$$\left.\begin{aligned} \mathbf{a}_1 &= a \cdot \mathbf{e}_2 \\ \mathbf{a}_2 &= \frac{a}{2}(\mathbf{e}_2 - \mathbf{e}_3) \\ \mathbf{a}_3 &= \frac{a}{2}(\mathbf{e}_1 + \mathbf{e}_2) \end{aligned}\right] \Rightarrow$$

But for atom 4, $\mathbf{a}_2$ has no atom at its end-point. 5.

$\boxed{\therefore \text{There's no three vectors that generate the lattice.}}$

(iii)



$\boxed{\text{It's a Bravais Lattice}}$

And
$$\boxed{\begin{aligned} \mathbf{a}_1 &= a\mathbf{e}_1 \\ \mathbf{a}_2 &= a\left(\frac{1}{2}\mathbf{e}_1 + \frac{\sqrt{3}}{2}\mathbf{e}_2\right) \end{aligned}}$$