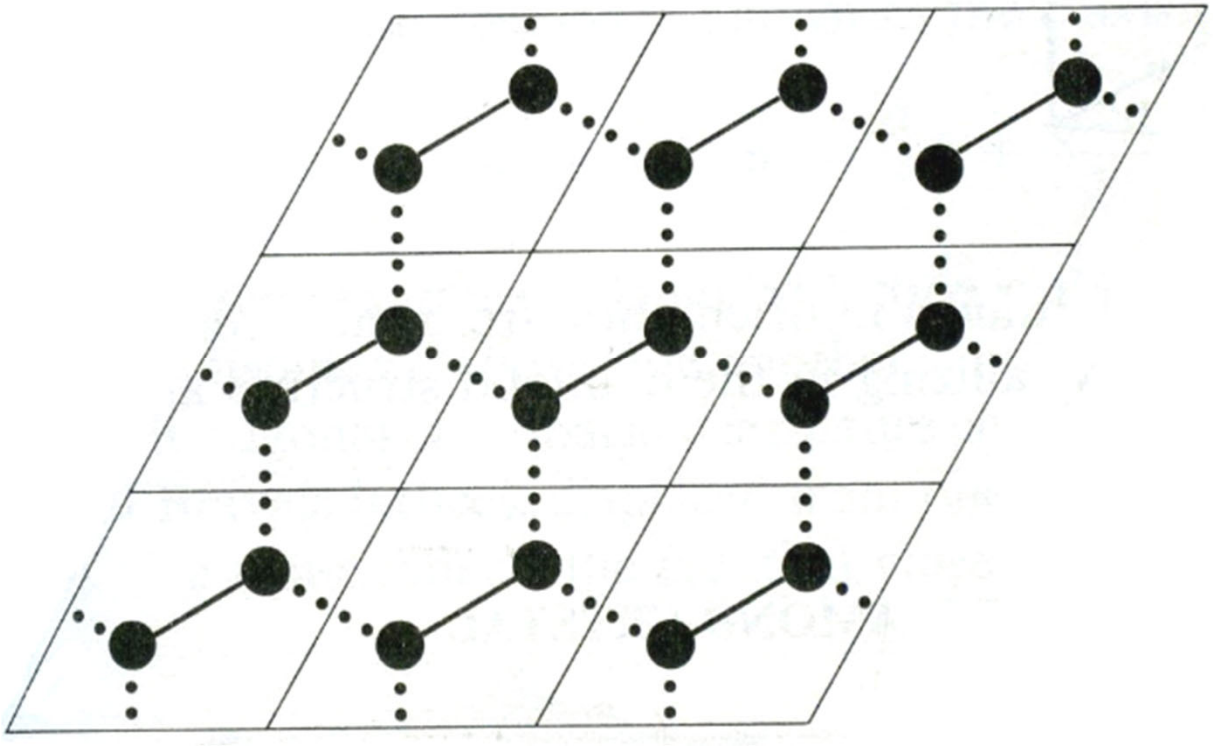
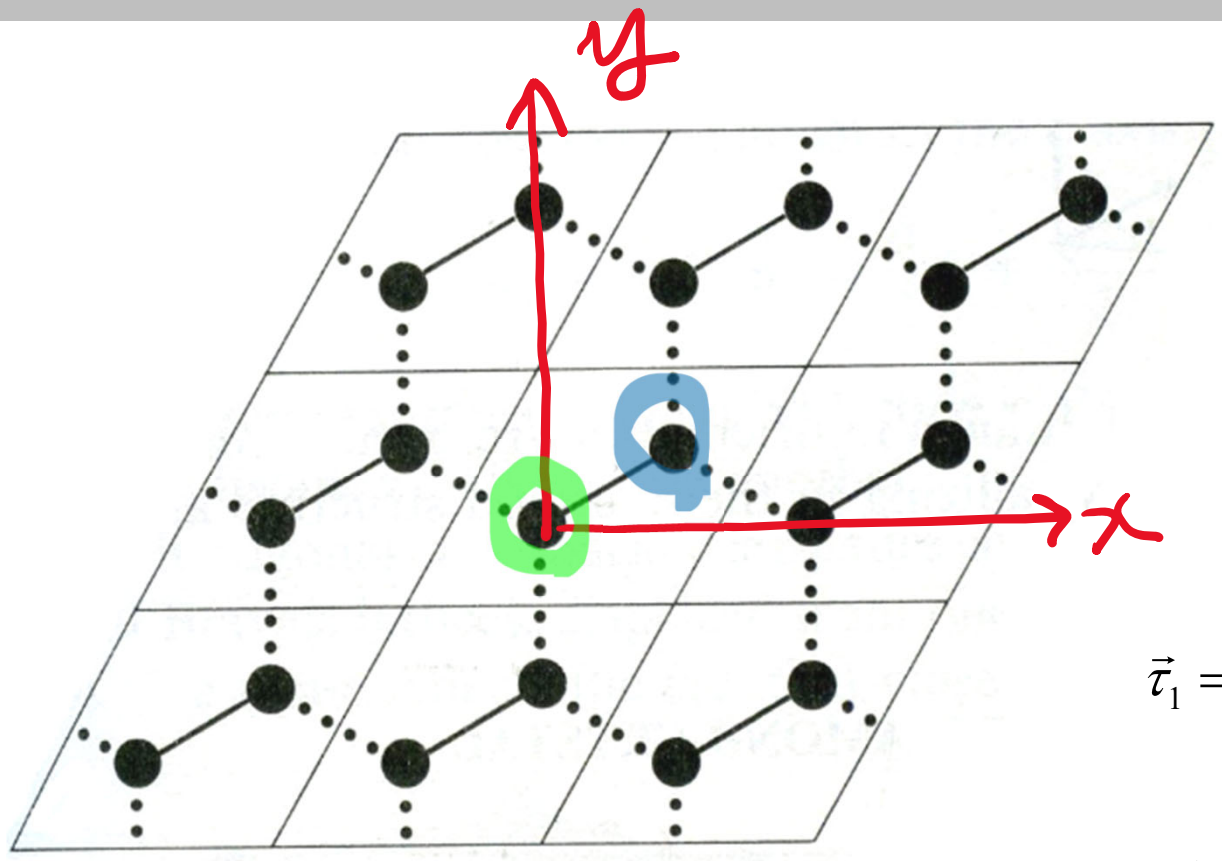
Honeycom structure in the triangular lattice



$$a = 2.47\text{Å},\ c = 3.35\text{Å}$$
$$d = 2.47\text{Å}$$
$$a = \sqrt{3}d$$

Honeycom structure in the triangular lattice



$$\vec{a}_1 = (a, 0, 0)$$

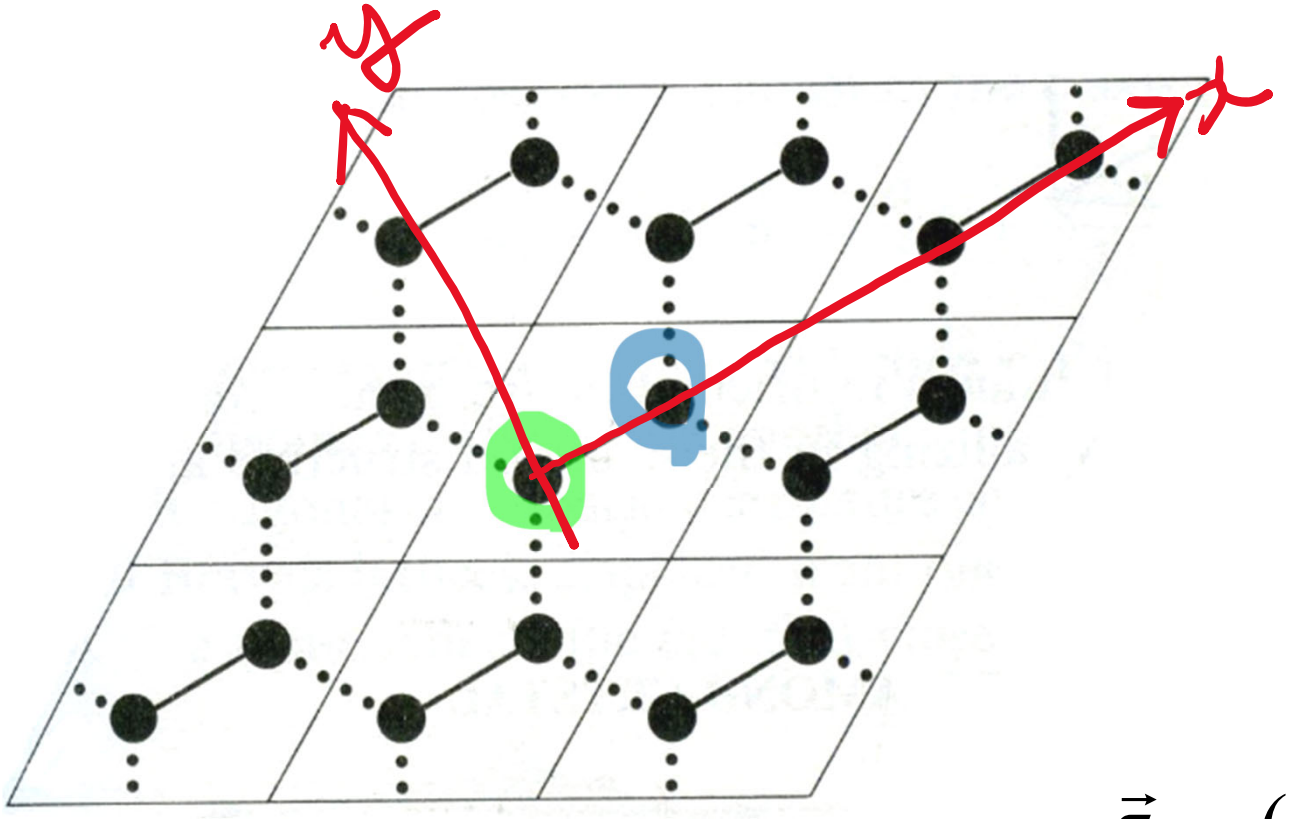
$$\vec{a}_2 = (\frac{1}{2}a, \frac{\sqrt{3}}{2}a, 0)$$

$$\vec{a}_3 = (0, 0, c)$$

$$\vec{\tau}_1 = (0,0,0) \ , \ \vec{\tau}_2 = (\frac{1}{2}a, \frac{\sqrt{3}}{6}a, 0) = \frac{1}{3}(\vec{a}_1 + \vec{a}_2)$$

$$\vec{R} = n\vec{a}_1 + l\vec{a}_2 + m\vec{a}_3$$

Honeycom structure in the triangular lattice



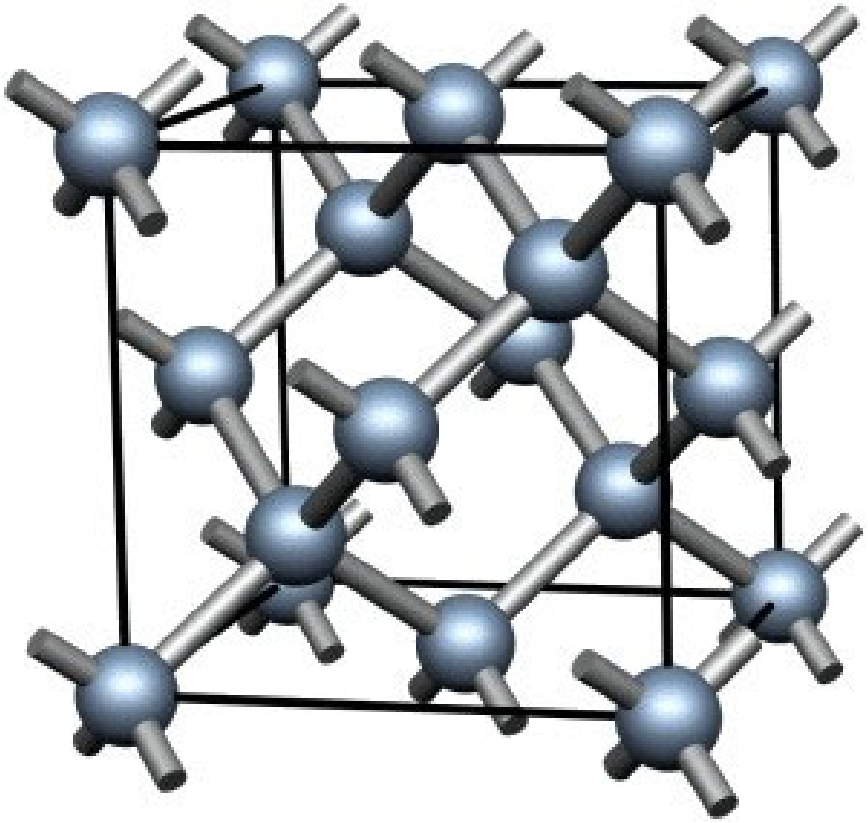
$$\vec{a}_1 = (\frac{\sqrt{3}}{2}a, -\frac{1}{2}a, 0)$$

$$\vec{a}_2 = (\frac{\sqrt{3}}{2}a, \frac{1}{2}a, 0)$$

$$\vec{a}_3 = (0, 0, c)$$

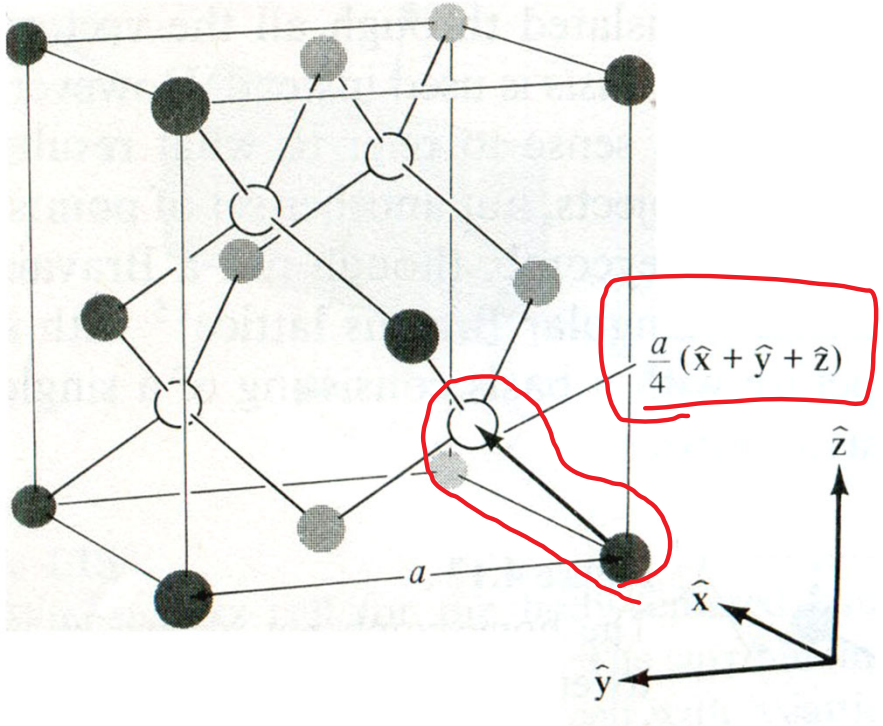
$$\vec{\tau}_1 = (0,0,0) \ , \ \vec{\tau}_2 = (\frac{a}{\sqrt{3}}, 0, 0)$$

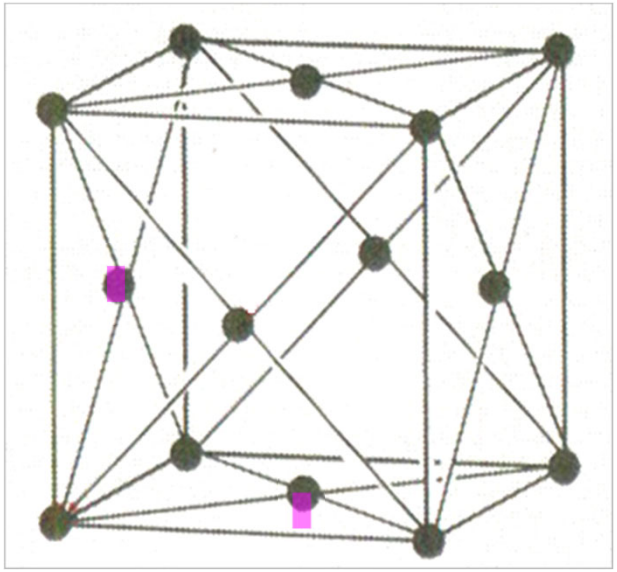
Diamond structure



4족 반도체의 대표구조,
Si 의 구조

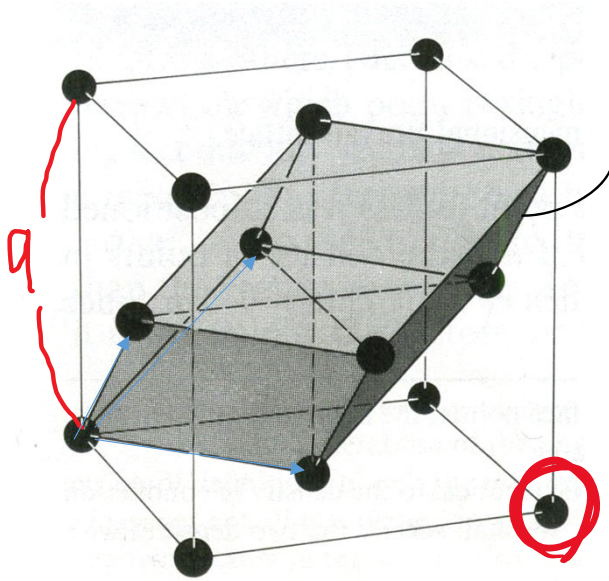
Diamond structure = FCC with two basis





FCC

Simple Cubic cell versus FCC cell.



$$\vec{a}_1 = \frac{a}{2}(\hat{i}+\hat{j})$$

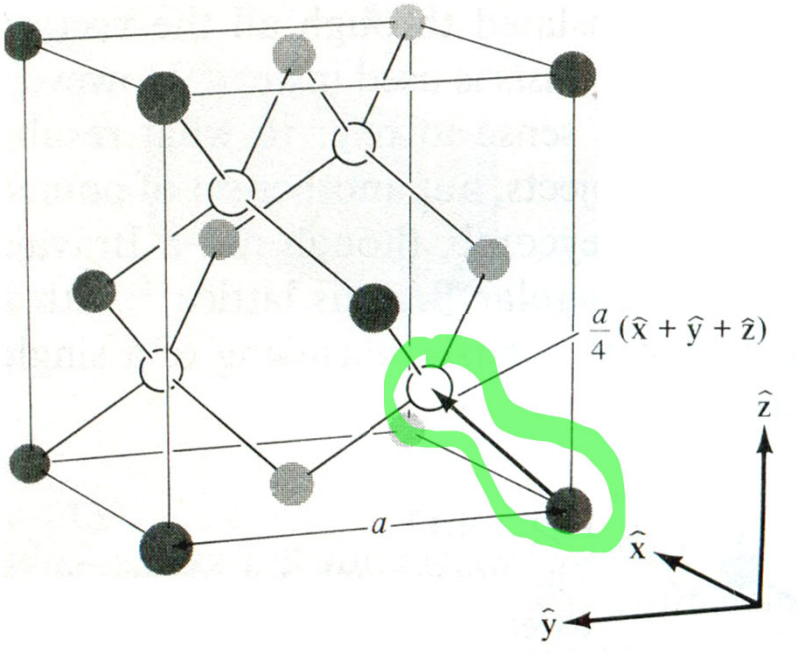
$$\vec{a}_2 = \frac{a}{2}(\hat{j}+\hat{k})$$

$$\vec{a}_3 = \frac{a}{2}(\hat{k}+\hat{i})$$

With two basis atoms

FCC

Diamond structure = FCC with two bases



$$\vec{a}_1 = \frac{a}{2}(\hat{i}+\hat{j})$$

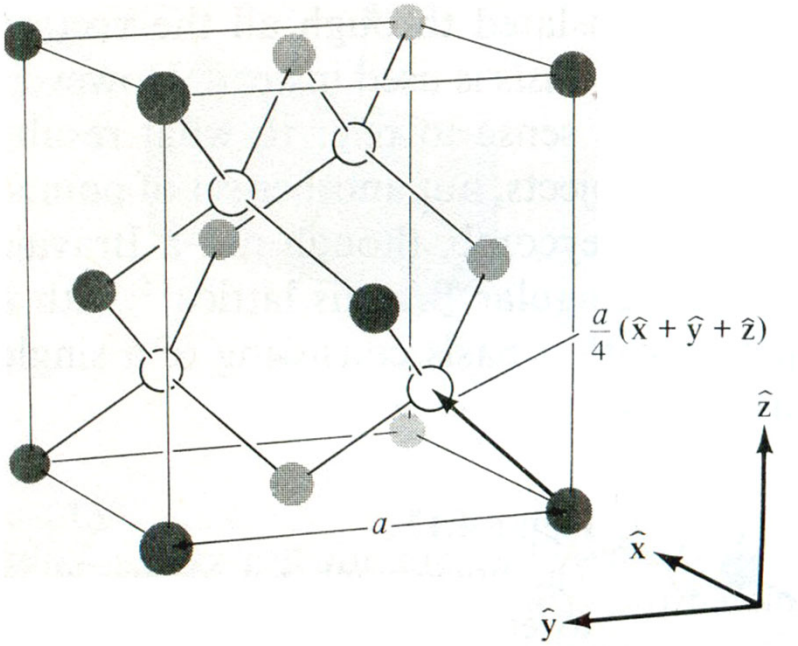
$$\vec{a}_2 = \frac{a}{2}(\hat{j}+\hat{k})$$

$$\vec{a}_3 = \frac{a}{2}(\hat{k}+\hat{i})$$

$$\vec{\tau}_1 = (0,0,0)$$

$$\vec{\tau}_2 = \frac{a}{4}(1,1,1) = \frac{1}{4}\left(\vec{a}_1 + \vec{a}_2 + \vec{a}_3\right)$$

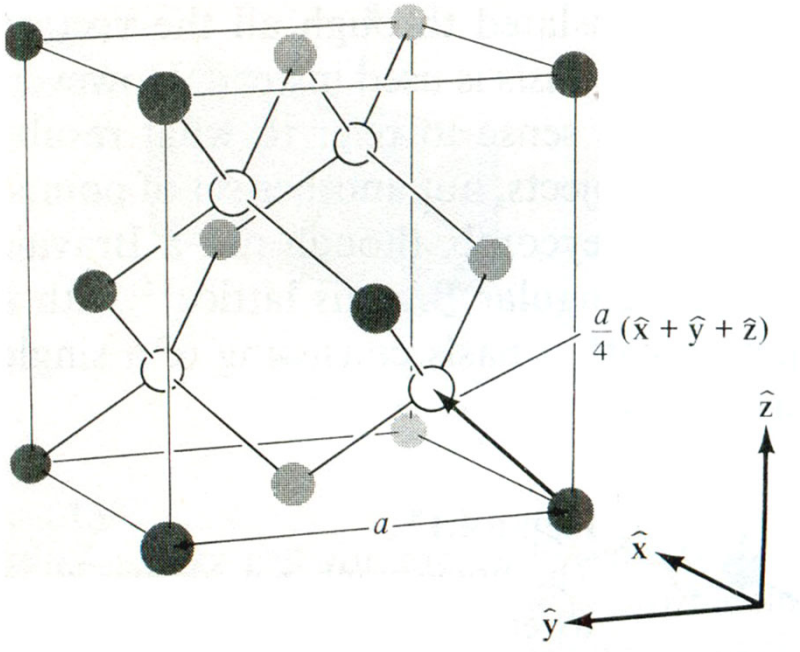
Diamond structure = SC with eight bases



$$\begin{cases} \vec{a}_1 = a\hat{x} \\ \vec{a}_2 = a\hat{y} \\ \vec{a}_3 = a\hat{z} \end{cases}$$

With 8 basis atoms

Diamond structure = SC with eight bases



Set up the coordinate system on your own choice of origin and axis.

[Q1] Describe the diamond structure in terms of FCC lattice with two basis atoms.

[Q2] Describe the diamond structure in terms of SC lattice with eight basis atoms.

Hamiltonian with a translational symmetry

The density functional Hamiltonian

$$\left(-\frac{1}{2}\nabla^2 + V(\vec{r})\right)\psi_{n,\mathbf{k}}(\mathbf{r}) = E_n(\mathbf{k})\psi_{n,\mathbf{k}}(\mathbf{r}) \quad , \quad \psi_{n,\mathbf{k}}(\mathbf{r}) = e^{i\vec{k}\cdot\vec{r}}u_{n,\mathbf{k}}(\vec{r})$$

$$\left(\frac{1}{2}(-i\nabla + \vec{k})^2 + V(\vec{r})\right)u_{n,\mathbf{k}}(\vec{r}) = E_n(\mathbf{k})u_{n,\mathbf{k}}(\vec{r})$$

$$V(\vec{r}) = \sum_{\mathbf{R}}^{\infty}\sum_{\tau=1}^{N_{basis}}\frac{-Z_\tau}{\left|\vec{r}-\vec{R}-\vec{\tau}\right|} + \int\frac{\rho(\vec{r}')}{\left|\vec{r}-\vec{r}'\right|}d^3\vec{r}' + V_{xc}[\rho(\vec{r})]$$

Hamiltonian with a translational symmetry

The density functional Hamiltonian

Uniform k-point sampling

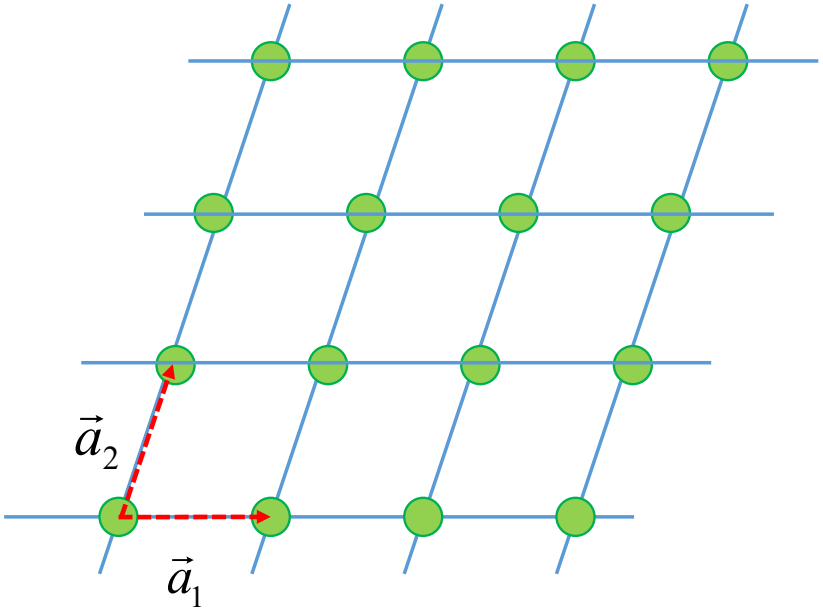
$$\left(\frac{1}{2}(-i\nabla+\vec{k})^2+V(\vec{r})\right)u_{n,\mathbf{k}}(\vec{r})=E_n(\mathbf{k})u_{n,\mathbf{k}}(\vec{r})$$

$$V(\vec{r})=\sum_{\mathbf{R}}^{\infty}\sum_{\tau=1}^{N_{basis}}\frac{-Z_\tau}{\left|\vec{r}-\vec{R}-\vec{\tau}\right|}+\int\frac{\rho(\vec{r}')}{\left|\vec{r}-\vec{r}'\right|}d^3\vec{r}'+V_{xc}[\rho(\vec{r})]$$

$$\rho(\vec{r})=\sum_{i=1}^{N_k}W(\vec{k})\sum_{n=1}^{N_{occp}}\left|e^{i\mathbf{k}\cdot\mathbf{r}}u_{n,\mathbf{k}}(\vec{r})\right|^2=\sum_{i=1}^{N_k}W(\vec{k})\sum_{n=1}^{N_{occp}}\left|u_{n,\mathbf{k}}(\vec{r})\right|^2$$

Lattice and reciprocal lattice

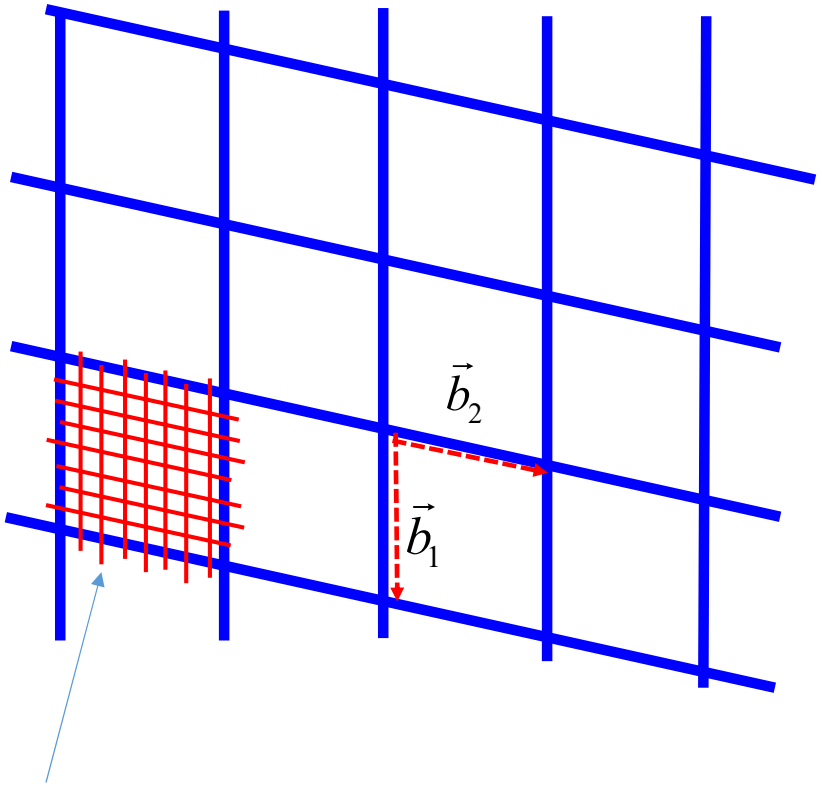
For example, a triangular lattice



$\vec{a}_1 = (a,0,0)$, $\vec{a}_2 = a(1/2, \sqrt{3}/2, 0)$, $\vec{a}_3 = (0,0,c)$

$$\vec{b}_1 = \frac{2\pi}{V}(\vec{a}_2 \times \vec{a}_3) = \frac{2\pi}{a}(1, -\frac{1}{\sqrt{3}}, 0)$$

$$\vec{b}_2 = \frac{2\pi}{V}(\vec{a}_3 \times \vec{a}_1) = \frac{2\pi}{a}(0, \frac{2}{\sqrt{3}}, 0)$$



Discrete uniform k-point sampling

Question

$$\int_{cell} \rho(\vec{r}) d^3\vec{r} =$$

Total energy of materials

$$E_{tot} = \sum_{n=1}^{occp} \sum_{\mathbf{k}} W(\vec{k}) \left\langle \psi_{n,\mathbf{k}} \left| -\frac{1}{2}\nabla^2 \right| \psi_{n,\mathbf{k}} \right\rangle + \frac{1}{2} \iint_{\infty} \frac{\rho(\vec{r})\rho(\vec{r}')}{\left|\vec{r}-\vec{r}'\right|} d^3\vec{r} d^3\vec{r}' + \int_{\infty} \rho(\vec{r}) \varepsilon_{xc}[\rho(\vec{r})] d^3\vec{r}$$

$$+ \int_{\infty} V(\vec{r})\rho(\vec{r}) d^3\vec{r}$$

$$+ \sum_{\lambda}^{\infty} \sum_{\mu}^{\infty} \frac{Z_\lambda Z_\mu}{\left|\vec{R}_\lambda - \vec{R}_\mu\right|}$$

So many infinite terms, How can we deal with these stuff ?

To derive the total energy per unit cell ?

Fourier transformation provides efficient ways.