

Empty Lattice Approximation for 100, simple cubic

$$E(\vec{k}, \vec{G}) = \frac{\hbar^2}{2m} (\vec{k} + \vec{G})^2 \quad \text{where } \vec{k} \text{ is in } 1^{\text{st}} \text{ B.Z.}$$

and \vec{G} = any reciprocal lattice vector

(1) \vec{k} is in [100] direction for this case

$$\rightarrow \vec{k} = (k, 0, 0)$$

(2) simple cubic lattice

$$\rightarrow \vec{G} = h\vec{b}_1 + l\vec{b}_2 + l\vec{b}_3$$

with $(h, l, l) = \text{integers}$

(this h is not the wave vector!)

$$\text{and } \vec{b}_1 = \frac{2\pi}{a} (1, 0, 0)$$

$$\vec{b}_2 = \frac{2\pi}{a} (0, 1, 0)$$

$$\vec{b}_3 = \frac{2\pi}{a} (0, 0, 1)$$

$$\text{so } \vec{G} = \frac{2\pi}{a} (h, l, l)$$

$$\begin{aligned} (\vec{k} + \vec{G})^2 &= (k_x + G_x, k_y + G_y, k_z + G_z) \cdot (k_x + G_x, k_y + G_y, k_z + G_z) \\ &= (k_x + G_x)^2 + (k_y + G_y)^2 + (k_z + G_z)^2 \\ &= \left(k + \frac{2\pi h}{a}\right)^2 + \left(0 + \frac{2\pi l}{a}\right)^2 + \left(0 + \frac{2\pi l}{a}\right)^2 \end{aligned}$$

Define x to go from 0 to 1 across the 1st BZ in the [100] direction.

$$x = \frac{k}{k_{\text{max}}} = \frac{k}{\frac{\pi}{a}} \rightarrow k = \frac{\pi}{a} x$$

$$E = \frac{\hbar^2}{2m} \left[\left(\frac{\pi}{a} x + \frac{2\pi h}{a}\right)^2 + \left(\frac{2\pi l}{a}\right)^2 + \left(\frac{2\pi l}{a}\right)^2 \right]$$

$$E = \frac{\hbar^2}{2m} \frac{\pi^2}{a^2} \left[(x + 2h)^2 + 4l^2 + 4l^2 \right]$$

E_{ref} = energy when $x = 1$ and $(h, l, l) = 0$

$$= \frac{\hbar^2}{2m} \frac{\pi^2}{a^2}$$

Empty lattice for 100 s.c., cont.

$$\frac{E}{E_{ref}} = (x+2h)^2 + 4k^2 + 4l^2$$

Plotted for various combinations of h, k, l

$$\text{up to } \frac{E}{E_{ref}} = 7$$

(Picking the hkl numbers ^{for simplicity} can be challenging. I did it with trial and error, and by thinking about the equation.

For example, the plots for (011) , $(0\bar{1}1)$, $(01\bar{1})$, and $(0\bar{1}\bar{1})$ will all be the same.)

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In[1]:= e[x_, h_, k_, l_] = (x+2h)^2 + 4k^2 + 4l^2
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Out[1]= 4 k^2 + 4 l^2 + (2 h + x)^2
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In[2]:= Plot[{e[x, 0, 0, 0], e[x, 1, 0, 0], e[x, -1, 0, 0], e[x, 0, 1, 0],  
e[x, 1, 1, 0], e[x, -1, 1, 0], e[x, 0, 1, 1]}, {x, -1, 1}, PlotRange -> {0, 9}]
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Out[2]=
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